METHOD

The present invention relates to polo-like kinases (PLKs) and small molecule inhibitors thereof. More specifically, the invention relates to a method for designing and identifying small molecule inhibitors using a homology model for PLK.

BACKGROUND TO THE INVENTION

The Polo-like kinase family consists of key cell cycle regulatory enzymes with integral roles in controlling entry into and progression through mitosis. Many tumour cells express high levels of PLK1 and are responsive to antisense oligonucleotides targeting this protein.

Initiation of mitosis requires activation of M-phase promoting factor (MPF), *i.e.* the complex between CDK1 and B-type cyclins [1]. The latter accumulate during the S and G2 phases of the cell cycle and promote the inhibitory phosphorylation of the MPF complex by WEE1, MIK1, and MYT1 kinases. At the end of the G2 phase, corresponding dephosphorylation by the dual-specificity phosphatase CDC25C triggers the activation of MPF [2]. In interphase, cyclin B localizes to the cytoplasm and becomes phosphorylated during prophase, followed by nuclear translocation. The nuclear accumulation of active MPF during prophase is thought to be important for initiating M-phase events [3]. However, nuclear MPF is kept inactive by WEE1 unless counteracted by CDC25C. The phosphatase CDC25C itself, localized to the cytoplasm during interphase, accumulates in the nucleus in prophase. The nuclear entry of both cyclin B and CDC25C are promoted through phosphorylation by PLK1 [4]. This kinase is thus an important regulator of M-phase initiation.

In humans, there exist three closely related polo-like kinases (PLKs) [5]. They contain a highly homologous N-terminal catalytic kinase domain and their C-termini contain two or three conserved regions, the polo boxes. The function of the polo boxes remains incompletely understood but polo box-dependent PLK1 activity is required for proper metaphase/anaphase transition and cytokinesis [6]. Of the three PLKs, PLK1 is the best characterized; it regulates a number of cell division cycle effects, including the onset of

mitosis, DNA-damage checkpoint activation, regulation of the anaphase promoting complex, phosphorylation of the proteasome, and centrosome duplication and maturation. Mammalian PLK2 (also known as SNK) and PLK3 (also known as PRK and FNK) were originally shown to be immediate early gene products. PLK3 kinase activity appears to peak during late S and G2 phase. It is also activated during DNA damage checkpoint activation and severe oxidative stress. PLK3 also plays an important role in the regulation of microtubule dynamics and centrosome function in the cell and deregulated PLK3 expression results in cell cycle arrest and apoptosis [7]. PLK2 is the least-well understood homologue of the three PLKs. Both PLK2 and PLK3 may have additional important post-mitotic functions [8].

The fact that human PLKs regulate some fundamental aspects of mitosis was shown by anti-PLK1 antibody microinjection of human tumour cells [9]. This treatment had no effect on DNA replication but impaired cell division. Cells were arrested in mitosis and showed abnormal distribution of condensed chromatin and monoastral microtubules nucleated from duplicated but unseparated centrosomes. By contrast, non-immortalized human cells arrested as single, mononucleated cells in G2. Moreover, when PLK1 function was blocked through adenovirus-mediated delivery of a dominant-negative gene, tumour-selective apoptosis in many tumour cell lines was observed, whereas again normal epithelial cells, although arrested in mitosis, escaped the mitotic catastrophe seen in tumour cells [10]. PLK1 activity is thus necessary for the functional maturation of centrosomes in late G2/early prophase and subsequent establishment of a bipolar spindle. Furthermore, these results suggest the presence in normal cells of a centrosome-maturation checkpoint that is sensitive to PLK1 impairment. Depletion of cellular PLK1 through the small interfering RNA (siRNA) technique also confirmed that this protein is required for multiple mitotic processes and completion of cytokinesis [11]. A potential therapeutic rationale for PLK inhibition is also suggested by work with PLK1-specific antisense oligonucleotides, which were shown to induce growth inhibition in cancer cells both *in vitro* and *in vivo* [12]. Constitutive expression of PLK1 in mammalian cells was shown to lead to malignant transformation [13]. Furthermore, overexpression of PLK1 is frequently observed in human tumours and

PLK1 expression is of prognostic value for patients suffering from various types of tumours [14-16].

Although the therapeutic potential of pharmacological PLK inhibition has been appreciated [17], very little has been reported to date concerning small-molecule PLK inhibitors that may be useful as drugs. The only characterized biochemical PLK1 inhibitor is scytonemin, a symmetric indolic marine natural product [18,19]. Scytonemin inhibits phosphorylation of CDC25C by recombinant PLK1 with an IC_{50} value of about 2 μM (at an ATP concentration of 10 μM). Inhibition is apparently reversible and the mechanism with respect to ATP of mixed-competitive mode. Similar potency against other protein serine/threonine- and dual specificity cell-cycle kinases, including MYT1, CHK1, CDK1/cyclin B, and PKC, was observed. Scytonemin showed pronounced anti-proliferative effects on various human cell lines in vitro.

The present invention seeks to elucidate small molecule PLK inhibitors, and in particular, provides a method for designing and identifying such inhibitors. The invention also seeks to elucidate further information on the 3-dimensional structure of the PLK binding domain and the nature of the binding interactions between PLK and such small molecule inhibitors.

STATEMENT OF INVENTION

The present invention relates to a homology model for PLK, and the use thereof in the indentification of small molecule PLK inhibitors.

As used herein, the term "model" refers to a structural model such as a three dimensional (3D) structural model (or representation thereof) comprising PLK. Preferably, the model comprising PLK is built from all or a portion of the structure co-ordinates presented in *Table 2*. The homology model of the invention enables candidate compounds to be identified that bind spatially and preferentially to PLK, particularly to the active site of PLK.

Aspects of the invention are presented in the accompanying claims and are further described in the following paragraphs.

DETAILED DESCRIPTION

ASSAYS BASED ON THE PLK1 HOMOLOGY MODEL

A first aspect of the invention relates to a method of screening for a modulator of PLK, wherein the method comprises using the structure co-ordinates of *Table 2.*

Since no experimental three-dimensional structures of PLK kinase domains are known, a PLK1 kinase domain homology model was constructed (*Example 1*). This model provides a plausible complex with the natural ligand ATP in the active site (*Figure 2*), as well as with two non-selective ATP-competitive kinase inhibitors, which were also found to inhibit PLK1, namely staurosporine [32] (IC_{50} w.r.t. PLK1 = 0.4 μM) and 4-[4-(4-methyl-2-methylamino-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol [33] (IC_{50} w.r.t. PLK1 = 4 μM) (*Figure 7*).

Of particular interest in the PLK1 kinase domain structure are Cys^{67} and Cys^{133}, both of which line the ATP binding site. Cys^{133} is located in the so-called hinge region, which is present in many kinases, and connects the N- and C-terminal lobes of the kinase domain. Its side chain projects away from the ATP-binding pocket, although its backbone NH and CO functions are probably involved in H-bonding with the purine system of ATP. The side chain of Cys^{67} on the PLK1 N-terminal lobe, on the other hand, points into the ATP-binding pocket and probably contributes directly to ATP binding *via* contacts with the ribose and/or triphosphate moieties. The position occupied by Cys^{67} in PLK1 is usually occupied by valine in other kinases and there contributes van der Waals contacts to ATP binding. A second unusual residue, Phe^{183}, which is commonly leucine in other kinases, also makes significant contributions to ATP binding through interactions with the purine system. These two key differences strongly suggest that they can be exploited in the generation of ATP-competitive inhibitors selective for PLK1. The presence of Cys^{67} in the pocket opens up the possibility that covalent or irreversible inhibitors could be developed.

As discussed above, Cys^{67} of PLK1 is of particular interest, since in the modelled PLK1-ATP complex structure it is positioned closely to the ribose ring of ATP (*Figure 4a*). More specifically, a close contact between the Cys^{67} thiol group and the 5'-O of the ribose portion of ATP is observed. A suitable adenosine-derived covalent inhibitor would thus be 5'-thioadenosine. Modelling (*Figure 4b*) of this compound into the active site of PLK1 suggests that a simple rotation of the C^{α}-C^{β} bond of Cys^{67} should accommodate this inhibitor in such a way as to bring the sulfur atoms of Cys^{67} and 5'-thioadenosine into disulfide-bonding distance without large perturbations of the bound adenine portion.

In order to test the hypothesis that Cys^{67} may indeed be involved in ATP binding by PLK1, the effect of non-specific thiol modifying agents such as thimerosal [34], N-ethylmaleimide, and iodoacetamide on PLK1 enzymatic activity was studied. All these reagents were found to inhibit CDC25C phosphorylation by PLK1 to some extent, indicating the involvement of Cys residues in enzymatic activity. The fact that such inhibition could be abolished in the presence of an excess of the reducing agent dithiothreitol, which specifically reduces disulfide bonds and competes with Cys thiol groups for thiol modifying agents [35], is consistent with this notion (*Example 8*). Adenosine derivatives were studied next (*Figure 5*). Unmodified adenosine did not inhibit PLK1 function at concentrations up to 0.2 mM, whereas 2'- and 5'-thioadenosines did. 5-Thioadenosine was about 3-fold more potent than its analogue 2'-thioadenosine, supporting the hypothesis that the 5'-OH of the ribose ring is better oriented to react with Cys^{67}. Again a lack of inhibition was observed in the presence of DTT. Kinetic analysis of PLK1 inhibition (*Example 14*) showed that with *e.g.* 5'-thioadenosine (*Figure 6*) this was dependent on ATP concentration but not competitive with ATP as would be the case for a reversible competitive ATP antagonist. The effects of the above thiol modifying reagents on a closely related serine/threonine kinase were also studied. Casein kinase II (CKII) was selected based on its sensitivity to certain inhibitors [36], *e.g.* wortmannin and LY294002 [37], which were also found to be capable of inhibiting PLK1 (IC_{50} with respect to PLK1 of < 0.1 μM and < 5 μM, respectively). No significant inhibition of CKII enzymatic activity was observed at concentrations up to 0.2 mM with thimerosal, N-ethylmaleimide, iodoacetamide,

adenosine, 2'-thioadenosine, or 5'-thioadenosine using the assay described in *Example 4*.

In summary, these results suggest that PLK-specific ATP antagonists can be developed that derive their potency and PLK selectivity from a combination of non-covalent binding to the unique ATP-binding pocket of PLK1 and covalent binding to the Cys^{67} thiol group.

Observations from modelled structures of PLK1 inhibitors

Studies were also carried out on purvalanol A and various flavonoid molecules. Further details of these studies are outlined in the accompanying examples section

The interactions of the potent Cdk2 inhibitors, staurosporine and purvalanol A with the PLK1 ATP cavity reveal why both of these inhibitors are non-selective for the two kinases. Staurosporine makes similar H-bond and van der Waals contacts in both structures, however is rotated by about 30° in the PLK1 structure with regards to Cdk2. The non-bonded energies for this inhibitor indicate a rough correlation with the observed IC50's as shown by the ludi energetic scores of 456 (H-bond 131, lipophilic 307) with PLK1 and 726 (H-bond 230, lipophilic 478) for Cdk2 (higher value indicates more favourable binding). Analysis of these scores indicates that the less favourable H-bond interactions in the PLK1 context contribute significantly to the lower inhibition. Unfavourable hydrophobic contacts result in rotation of the inhibitor and less optimal geometry of the hinge H-bonds.

Purvalanol A also makes similar contacts with both enzymes with H-bonds from the aniline N, a H-bond like interaction from the purine C, and favourable contacts with the L130 "gatekeeper" residue (*Figure 11A*) and thus demonstrates the structural basis for binding to both kinases. Again less optimal van der Waals contacts in the PLK1 case result in less optimal H-bond interactions with the interdomain connecting hinge.

Molecular docking of morin hydrate, the most potent in the flavonoid series, with the PLK1 homology model gives significant insight into the interactions of this compound

with ATP binding site. A binding mode that is consistent with known kinase inhibitor interactions was observed and the inhibitor makes numerous van der Waals and H-bond contacts (*Figure 11B*). These include the two hydroxyls on the aromatic section of the flavonoid ring acting as H-bond donors to the carbonyls of C133 and E131. The flavonoid ring makes van der Waals interactions with L130, the gatekeeper residue and the 1,3 substituted catechol ring, makes H-bond contacts to the sidechain of D194 and the backbone amide of A65. Analysis of the activities of the other structural homologues in this series (*Table 13*) indicates that this observed pose of morin bound to PLK1 is consistent with the structure-activity relationship. Datescetin, which is identical to morin except lacks the ortho-hydroxyl is inactive suggesting a significant role for the 3'-hyrdoxyl. Quercetin however has partial activity and contains the 3-hydroxyl but has no 1 hydroxyl. None of the other analogues in the series contains both the 1 and 3 position hydroxyls and therefore explains their loss of activity. The importance of both hydroxyl suggested by the SAR data is confirmed by the energetic contributions of H-bond interactions of these groups to the binding to the ATP cleft as shown in the docked structure. Placement of the hydroxyls on other positions in the ring would not allow optimal H-bond formation and thus indicates a structural rationale for their lack of potency in inhibiting PLK1 kinase activity.

Overall the postulated binding modes of the identified PLK1 inhibitors are energetically reasonable, consistent with observed structure-activity relationships and with the interactions of known kinase inhibitors. These results are therefore useful in design and synthesis of analogues of these structures which are optimized for PLK1 inhibition and selectivity.

Implications of the discovery of potent PLK1 kinase inhibitors

While the role of Cdks in the regulation of the cell cycle is very well established and comprehensively studied, PLKs clearly orchestrate events of the whole cell cycle [5]. However, very little is known about the physiological substrates for this class of enzymes. During mitosis and cytokinesis, PLKs are reported to associate with various structures involved in spindle formation and assembly including the centrosomes and kinetochores. Recent reports demonstrated the link between PLK1 in particular with

microtubule and microtubule-associated functions. Thus it is of a paramount importance to identify all the physiological substrates as well as all the posttranslational modifying enzymes for PLKs in order to understand their exact role in the cell cycle.

Over the last five years considerable efforts have been made in order to investigate the significance of PLK1 deregulation in the human health. A plethora of information is available strongly suggesting the oncogenicity of aberrantly expressed PLK1. As of yet, there is no direct evidence to prove the tumourogenic effects of the deregulated PLK1 activity and the challenge is therefore to determine the exact functions of PLK1 and subsequently determine the best routes for modulating this activity.

In the present study we sought to identify inhibitors of PLK1 *in vitro* and which could potentially applied to determine the cellular phenotype and consequences of reducing PLK1 kinase activity. The only inhibitor reported prior to this study is Scytonemin, a symmetric indolic marine natural product that is a micromolar non-specific ATP competitor [48]. Here we show for the first time that wortmannin is a very potent inhibitor of PLK1 while staurosporine and purvalanol A showed moderate inhibition.

Detailed examination indicated that while staurosporine inhibited PLK1 activity in an ATP dependent fashion, wortmannin inhibition was totally independent of ATP suggesting a different mode of binding. These results suggest a similar mode of inhibition to that reported previously for Phosphatidylinositol 3'OH kinase where wortmannin forms a covalent interaction with a Lysine residue (K833) positioned in the ATP binding pocket of the enzyme. Secondary structure analysis and homology modelling of the catalytic domain of PLK1 revealed the existence of a lysine residue (K82) projecting into the ATP binding cleft. It was therefore hypothesised that wortmannin covalently modifies this Lys residue and prevents ATP binding. It should be noted that previous reports clearly demonstrated that a single point mutation of K82 completely abolished the kinase activity of PLK1 since it required in the phosphotransfer step [49]. The observation from molecular modelling that the inhibitor docks in an orientation compatible with covalent interaction with K82, tolerates formation of the bond and energy minimisation without structural distortion and

interacts similarly to the PI3 kinase binding mode additionally confirms the validity of the homology structure. The high plausibility of this model therefore strongly supports the experimental data indicating irreversible binding of Wortmannin and is consistent with the hypothesis for reactivity with K82.

In addition to the identification of wortmannin, staurosporine, and purvalanol A as inhibitors of PLK1 kinase, the described flavonoid compounds are potential tool compounds for *in vitro* cellular screening in order to determine a phenotype of PLK1 inhibition. They also represent starting points for designing potent and selective small molecule inhibitors of this enzyme.

Preferred embodiments of the invention will now be described.

In one preferred embodiment of the invention, the method comprises the steps of:

(a) providing at least a portion of the structure co-ordinates of *Table 2*;

(b) employing at least a portion of the structure co-ordinates of *Table 2* to design or select or synthesise a putative modulator of PLK;

(c) contacting the putative modulator of PLK with PLK or a mutant, variant, homologue, derivative or fragment thereof, in the presence of a substrate of PLK; and

(d) determining whether said putative modulator of PLK modulates PLK.

In a preferred embodiment, at least a portion of the structure co-ordinates of *Table 2* and/or the putative modulator of PLK and/or the substrate are provided on a machine-readable data storage medium comprising a data storage material encoded with machine readable data.

In a preferred embodiment, the putative modulator of PLK is selected from a library of compounds. Preferably, the library is an *in silico* library. Suitable *in silico* libraries will be familiar to those skilled in the art, and include the Available Chemical Directory (MDL Inc), the Derwent World Drug Index (WDI), BioByteMasterFile, the National Cancer Institute database (NCI), and the Maybridge catalogue.

In another preferred embodiment, the putative modulator of PLK is selected from a database.

In another preferred embodiment, the putative modulator of PLK is designed *de novo*.

In yet another preferred embodiment, the putative modulator of PLK is designed from a known PLK modulator.

Preferably, the design or selection of the putative modulator of PLK is performed in conjunction with computer modelling.

In one particularly preferred embodiment, the putative modulator of PLK inhibits PLK activity.

More preferably, the PLK is PLK1.

In a further preferred embodiment, the putative modulator of PLK is useful in the prevention and/or treatment of a PLK related disorder.

Even more preferably, the PLK related disorder is a proliferative disorder.

More preferably still, the proliferative disorder is selected from cancer, leukemia, glomerulonephritis, rheumatoid arthritis, psoriasis and chronic obstructive pulmonary disorder.

A second aspect of the invention relates to an assay for a candidate compound capable of modulating PLK, said assay comprising the steps of:

(a) contacting said candidate compound with PLK;

(b) detecting whether said candidate compound forms associations with one or more amino acid residues corresponding to PLK amino acid residues L59, G60, A65, C67, A80, K82, L130, E131, C133, R135, F183 and D194.

In one preferred embodiment, said candidate compound is selected by performing rational drug design with a 3-dimensional model of PLK in conjunction with computer modelling.

In an even more preferred embodiment, the assay comprises detecting whether said candidate compound forms an association with the amino acid residue corresponding to PLK amino acid residue C67.

A third aspect of the invention relates to the use of a compound selected from the following:

(i) 5'-thioadenosine, or a derivative thereof;

(ii) staurosporine, wortmannin, purvalanol A, LY294002, quercetin, morin hydrate or derivatives thereof; and

(iii) 4-[4-(4-methyl-2-methylaminothiazol-5-yl)-pyrimidin-2-ylamino]-phenol; 4-[4-(2,4-dimethyl-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol or 4-[4-(2-amino-4-methyl-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol;

or a pharmaceutically acceptable salt thereof, in an assay for identifying candidate compounds capable of modulating PLK.

Preferably, the compound of (ii) is staurosporine, wortmannin, purvalanol A, LY294002, or morin hydrate. More preferably, the compound of (ii) is staurosporine, wortmannin, purvalanol A, even more preferably staurosporine or wortmannin.

Preferably, the assay is a competitive binding assay.

More preferably, the assay comprises contacting a candidate compound with PLK in the presence of a compound selected from:

(i) 5'-thioadenosine, or a derivative thereof;

(ii) staurosporine, wortmannin, purvalanol A, LY294002, quercetin, morin hydrate, or derivatives thereof; and

(iii) 4-[4-(4-methyl-2-methylaminothiazol-5-yl)-pyrimidin-2-ylamino]-phenol, 4-[4-(2,4-dimethyl-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol or 4-[4-(2-amino-4-methyl-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol;

or a pharmaceutically acceptable salt thereof, and detecting any change in the interaction between (i), (ii) or (iii) and PLK.

Another aspect of the invention relates to a computer for producing a three-dimensional representation of PLK wherein said computer comprises:

(a) a computer-readable data storage medium comprising a data storage material encoded with computer-readable data, wherein said data comprises the structure co-ordinates of *Table 2*;

(b) a working memory for storing instructions for processing said computer-readable data;

(c) a central-processing unit coupled to said working memory and to said computer-readable data storage medium for processing said computer-machine readable data into said three-dimensional representation; and

(d) a display coupled to said central-processing unit for displaying said three-dimensional representation.

Another aspect of the invention relates to a machine-readable data storage medium comprising a data storage material encoded with machine readable data, wherein the data is defined by at least a portion of the structure co-ordinates of *Table 2*.

A further aspect of the invention relates to the use of the above-described computer or machine readable data storage medium to predict the structure and/or function of potential modulators of PLK.

Another aspect relates to the use of at least a portion of the structure co-ordinates of *Table 2* to screen for modulators of PLK.

A further aspect relates to the use of at least a portion of the structure co-ordinates of *Table 2* to solve the structure of the crystalline form of any other protein with significant amino acid sequence homology to any functional domain of PLK.

Preferably, the structure of the crystalline form of any other protein with significant amino acid sequence homology to any functional domain of PLK is solved using molecular replacement.

Yet another aspect of the invention relates to the use of at least a portion of the structure co-ordinates of *Table 2* in molecular design techniques to design, select and synthesise modulators of PLK.

A further aspect of the invention relates to the use of at least a portion of the structure co-ordinates of *Table 2* in the development of compounds that can isomerise to reaction intermediates in the chemical reaction of a substrate or other compound that binds to PLK.

Another aspect of the invention relates to the use of at least a portion of the structure co-ordinates of *Table 2* to screen small molecule databases for chemical entities or compounds that modulate PLK.

PLK MODULATORS

A further aspect of the invention relates to a PLK modulator identified by the above-described method, or a candidate compound identified by the above-described assay.

Preferably, the PLK modulator or candidate compound of the invention inhibits PLK activity.

More preferably, the PLK modulator or candidate compound of the invention is capable of forming a covalent bond with the amino acid residue corresponding to PLK amino acid residue C67.

More preferably still, the PLK modulator or candidate compound of the invention is capable of forming a disulfide bond with the thiol group of the amino acid residue corresponding to PLK amino acid residue C67.

In one preferred embodiment, the PLK modulator or candidate compound of the invention is an irreversible antagonist.

The present invention permits the use of molecular design techniques to design, select and synthesise chemical entities and compounds, including PLK modulating compounds, capable of binding to PLK, in whole or in part.

By way of example, the structure co-ordinates of *Table 2* may be used to design compounds that bind to PLK and may alter the physical properties of the compounds (eg. solubility) or PLK itself. This invention may be used to design compounds that act as modulators, such as competitive inhibitors - of PLK by binding to all or a portion of the active site of PLK. Compounds may also be designed that act as non-competitive inhibitors of PLK. These non-competitive inhibitors may bind to all or a portion of PLK already bound to its substrate and may be more potent and specific than known PLK inhibitors that compete only for the PLK active site. Similarly, non-competitive inhibitors that bind to and inhibit PLK whether or not it is bound to another chemical entity may be designed using the structure co-ordinates of PLK described herein.

The present invention may also allow the development of compounds that can isomerise to reaction intermediates in the chemical reaction of a substrate or other compound that binds to PLK. Thus, the time-dependent analysis of structural changes in PLK during its interaction with other molecules may be performed. The reaction intermediates of PLK may also be deduced from the reaction product in co-complex with PLK. Such information is especially useful to design improved analogues of known PLK modulators or to design new PLK modulators based on the reaction intermediates of the PLK enzyme and PLK-modulator complex. This may provide a new route for designing PLK modulators with high specificity and stability. Preferably, this provides a new route for designing PLK modulators with high specificity, high stability and low toxicity.

Small molecule databases or candidate compounds may be screened for chemical entities or compounds that can bind in whole, or in part, to PLK. Thus, in a preferred

embodiment, the putative PLK modulator is from a library of compounds or a database. In this screening, the quality of fit of such entities or compounds to the binding site may be judged by various methods – such as shape complementarity or estimated interaction energy (Meng, E. C. *et al.*, *J. Comp. Chem.*, 13, pp. 505-524 (1992)).

The structure co-ordinates of *Table 2*, or portions thereof, may also be useful in solving the structure of crystal forms of PLK. They may also be used to solve the structure of PLK mutants, PLK variants, PLK homologues, PLK derivatives, PLK fragments and PLK complexes.

Preferably, the structure co-ordinates of *Table 2* may be used to solve the structure of the crystalline form of proteins having significant amino acid sequence homology to any functional domain of PLK. By way of example, molecular replacement may be used. In this method, the unknown crystal structure, whether it is a crystal form of PLK, a PLK mutant, a PLK variant, a PLK homologue (eg. another protein with significant amino acid sequence homology to any functional domain of PLK), a PLK derivative, a PLK fragment or a PLK co-complex may be determined using the PLK structure co-ordinates of the present invention. This method will provide a more accurate structural form for the unknown crystal more quickly and efficiently than attempting to determine such information *ab initio*.

In a preferred embodiment of the present invention, the PLK crystal of unknown structure further comprises an entity bound to the PLK protein or a portion thereof, for example, an entity that is an inhibitor of PLK.

The crystal structures of such complexes may be solved by molecular replacement or in combination with MAD (Multiwavelength Anomalous Dispersion) and/or MIRAS (Multiple Isomorphous Replacement with Anomalous Scattering) procedures - and compared with that of wild-type PLK. Potential sites for modification within the binding sites of the enzyme may thus be identified. This information provides an additional tool for determining the most efficient binding interactions, for example, increased hydrophobic interactions, between PLK and a chemical entity or compound.

The structures and complexes of PLK may be refined using computer software - such as X-PLOR (Meth. Enzymol., vol. 114 & 115, H. W. Wyckoff et al., eds., Academic Press (1985)), MLPHARE (Collaborative computational project Number 4. The CCP4 Suite: Programs for Protein Crystallography (1994) Acta Crystallogr. D 50, 760-763) and SHARP [De La Fortelle, E. & Bricogne, G. Maximum-likelihood heavy-atom parameters refinement in the MIR and MAD methods (1997) Methods Enzymol. 276, 472-494). Preferably, the complexes are refined using the program CNS (Brünger *et al.* (1998) *Acta Crystallogr.* D 54, 905-921). During the final stages of refinement water molecules, ions and inhibitor molecules may be inserted in the structure. This information may thus be used to optimise known classes of PLK modulators, eg. PLK inhibitors, and more importantly, to design and synthesise novel classes of PLK modulators.

The overall figure of merit may be improved by iterative solvent flattening, phase combination and phase extension with the program SOLOMON [Abrahams, J. P. & Leslie, A. G. W. Methods used in structure determination of bovine mitochondrial F1 ATPase. (1996) Acta Crystallogr. D 52, 110-119].

The structure co-ordinates of the homology model of the present invention may also facilitate the identification of related proteins or enzymes analogous to PLK in function, structure or both, thereby further leading to novel therapeutic modes for treating or preventing PLK related diseases.

The design of compounds that bind to or modulate PLK according to the present invention generally involves consideration of two factors. Firstly, the compound must be capable of physically and structurally associating with PLK. Non-covalent molecular interactions important in the association of PLK with its substrate may include hydrogen bonding, van der Waals and hydrophobic interactions. Secondly, the compound must be able to assume a conformation that allows it to associate with PLK. Although certain portions of the compound may not directly participate in the association with PLK, those portions may still influence the overall conformation of the molecule. This may have a significant impact on potency. Such conformational

requirements include the overall three-dimensional structure and orientation of the chemical entity or compound in relation to all or a portion of a binding site of PLK, or the spacing between functional groups of a compound comprising several chemical entities that directly interact with PLK.

The potential modulating or binding effect of a chemical compound on PLK may be analysed prior to its actual synthesis and testing by the use of computer modelling techniques. If the theoretical structure of the given compound suggests insufficient interaction and association with PLK, then synthesis and testing of the compound may be obviated. However, if computer modelling indicates a strong interaction, the molecule may be synthesised and tested for its ability to bind to PLK and modulate (eg. inhibit) using the fluorescent substrate assay of Thornberry *et al.* (2000) *Methods Enzymol.* 322, pp 100-110. In this manner, synthesis of inactive compounds may be avoided.

A modulating or other binding compound of PLK may be computationally evaluated and designed by means of a series of steps in which chemical entities or candidate compounds are screened and selected for their ability to associate with PLK.

A person skilled in the art may use one of several methods to screen chemical entities or candidate compounds for their ability to associate with PLK and more particularly with the individual binding sites of PLK. This process may begin by visual inspection of, for example, the active site on the computer screen based on the PLK co-ordinates of the present invention. Selected chemical entities or candidate compounds may then be positioned in a variety of orientations, or docked, with PLK. Docking may be accomplished using software such as Quanta and Sybyl, followed by energy minimisation and molecular dynamics with standard molecular mechanics force fields - such as CHARMM and AMBER.

Specialised computer programs may also assist in the process of selecting chemical entities or candidate compounds. These include but are not limited to MCSS (Miranker and Karplus (1991) Proteins: Structure, Function and Genetics, 11, pp. 29-34); GRID

(Goodford (1985) J. Med. Chem., 28, pp. 849-857) and AUTODOCK (Goodsell and Olsen (1990), Proteins: Structure. Function, and Genetics, 8, pp. 195-202.

Once suitable chemical entities or candidate compounds have been selected, they may be assembled into a single compound, such as a PLK modulator. Assembly may proceed by visual inspection of the relationship of the chemical entities or candidate compounds in relation to the structure co-ordinates of PLK. This may be followed by manual model building using software - such as Quanta, Sybyl, O, HOOK or CAVEAT [Jones, T. A., Zou, J. Y., Cowan, S. W. & Kjeldgaard, M. Improved methods for building protein models in electron density maps and the location of errors in these models (1991) Acta Crystallogr. A 47, 110-119].

Refinement of the model may be carried out using the program CNS [Brünger, A. T. et al. Crystallography & NMR System: A new software suite for macromolecular structure determination. (1998) Acta Crystallogr. D 54, 905-921].

Various programs may be used by a skilled person to connect the individual chemical entities or candidate compounds, such as 3D Database systems (Martin (1992) *J. Med. Chem.*, 35, pp. 2145-2154) and CAVEAT (Bartlett *et al.* (1989) *Royal Chem. Soc.* 78, pp. 182-196).

Rather than build a PLK inhibitor one chemical entity at a time, modulating or other PLK binding compounds may be designed as a whole or *de novo* using either an empty binding site or optionally including some portion(s) of a known inhibitor(s). Such compounds may be designed using programs that may include but are not limited to LEGEND (Nishibata and Itai (1991) Tetrahedron, 47, p. 8985) and LUDI (Bohm (1992) *J. Comp. Aid. Molec. Design*, 6, pp. 61-78).

Other molecular modelling techniques may also be employed in accordance with this invention – such as those described by Cohen et al., J. Med. Chem., 33, pp. 883-894 (1990); Navia and Murcko (1992) Current Opinions in Structural Biology, 2, pp. 202-210 (1992).

Once a compound has been designed or selected by the above methods, the efficiency with which that compound may bind to PLK may be computationally evaluated. Specific computer software may be used to evaluate the efficiency of binding (eg. to evaluate compound deformation energy and electrostatic interaction), such as QUANTA/CHARMM (Accelrys Inc., USA) and Insight II/Discover (Biosym Technologies Inc., San Diego, Calif., USA). These programs may be implemented, for instance, using a suitable workstation. Other hardware systems and software packages will be known to those persons skilled in the art.

Once a PLK-modulating compound has been selected or designed, as described above, substitutions may be made (eg. in atoms or side groups) to improve or modify the binding properties. The substitutions may be conservative ie. the replacement group may have approximately the same size, shape, hydrophobicity and charge as the original group. Such substituted chemical compounds may then be analysed for efficiency of binding to PLK by the same computer methods described above.

Candidate compounds and modulators of PLK etc. which are identified using the methods of the present invention may be screened in assays. Screening can be, for example *in vitro*, in cell culture, and/or *in vivo*. Biological screening assays preferably centre on activity-based response models, binding assays (which measure how well a compound binds), and bacterial, yeast and animal cell lines (which measure the biological effect of a compound in a cell). The assays can be automated for high capacity-high throughput screening (HTS) in which large numbers of compounds can be tested to identify compounds with the desired activity.

Current screening technologies are described in Handbook of Drug Screening, edited by Ramakrishna Seethala, Prabhavathi B. Fernandes. New York, NY, Marcel Dekker, (2001).

MODULATING PLK

As herein, the term "modulating" or "modulates" refers to preventing, suppressing, inhibiting, alleviating, restorating, elevating, increasing or otherwise affecting PLK.

The term "PLK modulator" may refer to a single entity or a combination of entities.

The PLK modulator may be an antagonist or an agonist of PLK.

As used herein, the term "agonist" means any entity, which is capable of interacting (eg. binding) with PLK and which is capable of increasing a proportion of the PLK that is in an active form, resulting in an increased biological response.

As used herein, the term "antagonist" means any entity, which is capable of interacting (eg. binding) with PLK and which is capable of decreasing (eg. inhibiting) a proportion of the PLK that is in an active form, resulting in a decreased biological response.

Preferably, the PLK modulators of the present invention are antagonists of PLK.

The modulator of PLK may be an organic compound or other chemical. The modulator of PLK may be a compound, which is obtainable from or produced by any suitable source, whether natural or artificial. The modulator of PLK may be an amino acid molecule, a polypeptide, or a chemical derivative thereof, or a combination thereof. The modulator of PLK may even be a polynucleotide molecule, which may be a sense or an anti-sense molecule. The modulator of PLK may even be an antibody.

The modulator of PLK may be designed or obtained from a library of compounds, which may comprise peptides, as well as other compounds, such as small organic molecules.

By way of example, the modulator of PLK may be a natural substance, a biological macromolecule, or an extract made from biological materials such as bacteria, fungi, or animal (particularly mammalian) cells or tissues, an organic or an inorganic molecule, a synthetic agent, a semi-synthetic agent, a structural or functional mimetic, a peptide, a peptidomimetic, a derivatised agent, a peptide cleaved from a whole protein, or a peptide synthesised synthetically (such as, by way of example, either using a peptide synthesiser or by recombinant techniques or combinations thereof, a recombinant agent,

an antibody, a natural or a non-natural agent, a fusion protein or equivalent thereof and mutants, derivatives or combinations thereof).

Typically, the modulator of PLK will be an organic compound. Typically, the organic compounds will comprise two or more hydrocarbyl groups. Here, the term "hydrocarbyl group" means a group comprising at least C and H and may optionally comprise one or more other suitable substituents. Examples of such substituents may include halo-, alkoxy-, nitro-, an alkyl group, a cyclic group etc. In addition to the possibility of the substituents being a cyclic group, a combination of substituents may form a cyclic group. If the hydrocarbyl group comprises more than one C then those carbons need not necessarily be linked to each other. For example, at least two of the carbons may be linked *via* a suitable element or group. Thus, the hydrocarbyl group may contain hetero atoms. Suitable hetero atoms will be apparent to those skilled in the art and include, for instance, sulphur, nitrogen and oxygen. For some applications, preferably the modulator of PLK comprises at least one cyclic group. The cyclic group may be a polycyclic group, such as a non-fused polycyclic group. For some applications, the modulator of PLK comprises at least the one of said cyclic groups linked to another hydrocarbyl group.

The modulator of PLK may contain halo groups, for example, fluoro, chloro, bromo or iodo groups, or one or more of alkyl, alkoxy, alkenyl, alkylene and alkenylene groups, each of which may be branched or unbranched.

The modulator of PLK may be a structurally novel modulator of PLK, or may be an analogue of a known modulator of PLK.

Preferably, the PLK modulators have improved properties over those previously available, for example, fewer side effects.

The modulator of PLK may be a mimetic, or may be chemically modified.

The modulator of PLK may be capable of displaying other therapeutic properties.

The modulator of PLK may be used in combination with one or more other pharmaceutically active agents. If combinations of active agents are administered, then they may be administered simultaneously, separately or sequentially.

CANDIDATE COMPOUNDS

As used herein, the term "candidate compound" includes, but is not limited to, a compound which may be obtainable from or produced by any suitable source, whether natural or not.

The candidate compound may be designed or obtained from a library of compounds, which may comprise peptides, as well as other compounds, such as small organic molecules and particularly new lead compounds. By way of example, the candidate compound may be a natural substance, a biological macromolecule, or an extract made from biological materials - such as bacteria, fungi, or animal (particularly mammalian) cells or tissues, an organic or an inorganic molecule, a synthetic candidate compound, a semi-synthetic candidate compound, a structural or functional mimetic, a peptide, a peptidomimetic, a derivatised candidate compound, a peptide cleaved from a whole protein, or a peptide synthesised synthetically, for example, either using a peptide synthesiser or by recombinant techniques or combinations thereof, a recombinant candidate compound, a natural or a non-natural candidate compound, a fusion protein or equivalent thereof and mutants, derivatives or combinations thereof. The candidate compound may even be a compound that is a modulator of PLK, such as a known inhibitor of PLK, that has been modified in some way eg. by recombinant DNA techniques or chemical synthesis techniques.

Typically, the candidate compound will be prepared by recombinant DNA techniques and/or chemical synthesis techniques.

Once a candidate compound capable of interacting PLK has been identified, further steps may be carried out to select and/or to modify the candidate compounds and/or to modify existing compounds, such that they are able to modulate PLK.

In one aspect, the modulator of PLK may act as a model (for example, a template) for the development of other compounds.

A further aspect relates to the use of candidate compounds or PLK modulators identified by the assays and methods of the invention in one or more model systems, for example, in a biological model, a disease model, or a model for PLK inhibition. Such models may be used for research purposes and for elucidating further details of the biological, physicochemical, pharmacological and/or pharmacokinetic activity of a particular candidate compound. By way of example, the candidate compounds or PLK modulators of the present invention may be used in biological models or systems in which the cell cycle is known to be of particular significance, e.g. in models relating to cell fertilization, especially in animals.

MIMETIC

As used herein, the term "mimetic" relates to any chemical which includes, but is not limited to, a peptide, polypeptide, antibody or other organic chemical which has the same qualitative activity or effect as a known compound. That is, the mimetic is a functional equivalent of a known compound.

CHEMICAL SYNTHESIS METHODS

Preferably, the modulator of PLK of the present invention may be prepared by chemical synthesis techniques.

It will be apparent to those skilled in the art that sensitive functional groups may need to be protected and deprotected during synthesis of a compound of the invention. This may be achieved by conventional techniques, for example as described in "Protective Groups in Organic Synthesis" by T W Greene and P G M Wuts, John Wiley and Sons Inc. (1991), and by P.J.Kocienski, in "Protecting Groups", Georg Thieme Verlag (1994).

It is possible during some of the reactions that any stereocentres present could, under certain conditions, be racemised, for example if a base is used in a reaction with a substrate having an having an optical centre comprising a base-sensitive group. This is possible during e.g. a guanylation step. It should be possible to circumvent potential

problems such as this by choice of reaction sequence, conditions, reagents, protection/deprotection regimes, etc. as is well-known in the art.

The compounds and salts may be separated and purified by conventional methods.

Separation of diastereomers may be achieved by conventional techniques, e.g. by fractional crystallisation, chromatography or H.P.L.C. of a stereoisomeric mixture of a compounds or suitable salts or derivatives thereof. An individual enantiomer of a compound may also be prepared from a corresponding optically pure intermediate or by resolution, such as by H.P.L.C. of the corresponding racemate using a suitable chiral support or by fractional crystallisation of the diastereomeric salts formed by reaction of the corresponding racemate with a suitably optically active acid or base.

PLK, modulators of PLK or variants, homologues, derivatives, fragments or mimetics thereof may be produced using chemical methods to synthesise the PLK or the modulator of PLK in whole or in part. For example, a PLK peptide or a modulator of PLK that is a peptide can be synthesised by solid phase techniques, cleaved from the resin, and purified by preparative high performance liquid chromatography (e.g., Creighton (1983) Proteins Structures And Molecular Principles, WH Freeman and Co, New York NY). The composition of the synthetic peptides may be confirmed by amino acid analysis or sequencing (e.g., the Edman degradation procedure; Creighton, *supra*).

Synthesis of peptides (or variants, homologues, derivatives, fragments or mimetics thereof) may be performed using various solid-phase techniques (Roberge JY *et al* (1995) Science 269: 202-204) and automated synthesis may be achieved, for example, using the ABI 43 1 A Peptide Synthesizer (Perkin Elmer) in accordance with the instructions provided by the manufacturer. Additionally, the amino acid sequences comprising the modulator of PLK, may be altered during direct synthesis and/or combined using chemical methods with a sequence from other subunits, or any part thereof, to produce a variant modulator of PLK.

CHEMICAL MODIFICATION

In one embodiment, the modulator of PLK may be a chemically modified modulator of PLK. The chemical modification of a modulator of PLK may either enhance or reduce interactions between the modulator of PLK and the target, such as hydrogen bonding interactions, charge interactions, hydrophobic interactions, van der Waals interactions or dipole interactions.

PROCESS

Another aspect of the invention relates to a process comprising the steps of:

(a) performing the method according to the invention, or an assay according to the invention;

(b) identifying one or more modulators of PLK; and

(c) preparing a quantity of said one or more PLK modulators.

A further aspect of the invention relates to a process comprising the steps of:

(a) performing the method according to the invention, or an assay according to the invention;

(b) identifying one or more PLK modulators; and

(c) preparing a pharmaceutical composition comprising said one or more identified PLK modulators.

A further aspect relates to a process comprising the steps of:

(a) performing the method according to the invention, or an assay according to the invention;

(b) identifying one or more PLK modulators;

(c) modifying said one or more PLK modulators; and

(d) optionally preparing a pharmaceutical composition comprising said one or more PLK modulators.

PHARMACEUTICAL COMPOSITIONS

Another aspect of the invention relates to a pharmaceutical composition comprising a PLK modulator or candidate compound of the invention and a pharmaceutically

acceptable carrier, diluent, excipient or adjuvant or any combination thereof. Even though the PLK modulators or candidate compounds (including their pharmaceutically acceptable salts, esters and pharmaceutically acceptable solvates) can be administered alone, they will generally be administered in admixture with a pharmaceutical carrier, excipient or diluent, particularly for human therapy. The pharmaceutical compositions may be for human or animal usage in human and veterinary medicine.

Examples of such suitable excipients for the various different forms of pharmaceutical compositions described herein may be found in the "Handbook of Pharmaceutical Excipients, 2nd Edition, (1994), Edited by A Wade and PJ Weller.

Acceptable carriers or diluents for therapeutic use are well known in the pharmaceutical art, and are described, for example, in Remington's Pharmaceutical Sciences, Mack Publishing Co. (A. R. Gennaro edit. 1985).

Examples of suitable carriers include lactose, starch, glucose, methyl cellulose, magnesium stearate, mannitol, sorbitol and the like. Examples of suitable diluents include ethanol, glycerol and water.

The choice of pharmaceutical carrier, excipient or diluent can be selected with regard to the intended route of administration and standard pharmaceutical practice. The pharmaceutical compositions may comprise as, or in addition to, the carrier, excipient or diluent any suitable binder(s), lubricant(s), suspending agent(s), coating agent(s), solubilising agent(s).

Examples of suitable binders include starch, gelatin, natural sugars such as glucose, anhydrous lactose, free-flow lactose, beta-lactose, corn sweeteners, natural and synthetic gums, such as acacia, tragacanth or sodium alginate, carboxymethyl cellulose and polyethylene glycol.

Examples of suitable lubricants include sodium oleate, sodium stearate, magnesium stearate, sodium benzoate, sodium acetate, sodium chloride and the like.

Preservatives, stabilizers, dyes and even flavoring agents may be provided in the pharmaceutical composition. Examples of preservatives include sodium benzoate, sorbic acid and esters of p-hydroxybenzoic acid. Antioxidants and suspending agents may be also used.

SALTS/ESTERS

The PLK modulators or candidate compounds of the present invention can be present as salts or esters, in particular pharmaceutically acceptable salts or esters.

Pharmaceutically acceptable salts of the PLK modulators or candidate compounds of the invention include suitable acid addition or base salts thereof. A review of suitable pharmaceutical salts may be found in Berge et al, J Pharm Sci, 66, 1-19 (1977). Salts are formed, for example with strong inorganic acids such as mineral acids, e.g. sulphuric acid, phosphoric acid or hydrohalic acids; with strong organic carboxylic acids, such as alkanecarboxylic acids of 1 to 4 carbon atoms which are unsubstituted or substituted (e.g., by halogen), such as acetic acid; with saturated or unsaturated dicarboxylic acids, for example oxalic, malonic, succinic, maleic, fumaric, phthalic or tetraphthalic; with hydroxycarboxylic acids, for example ascorbic, glycolic, lactic, malic, tartaric or citric acid; with aminoacids, for example aspartic or glutamic acid; with benzoic acid; or with organic sulfonic acids, such as (C_1-C_4)-alkyl- or aryl-sulfonic acids which are unsubstituted or substituted (for example, by a halogen) such as methane- or p-toluene sulfonic acid.

Esters are formed either using organic acids or alcohols/hydroxides, depending on the functional group being esterified. Organic acids include carboxylic acids, such as alkanecarboxylic acids of 1 to 12 carbon atoms which are unsubstituted or substituted (e.g., by halogen), such as acetic acid; with saturated or unsaturated dicarboxylic acid, for example oxalic, malonic, succinic, maleic, fumaric, phthalic or tetraphthalic; with hydroxycarboxylic acids, for example ascorbic, glycolic, lactic, malic, tartaric or citric acid; with aminoacids, for example aspartic or glutamic acid; with benzoic acid; or with organic sulfonic acids, such as (C_1-C_4)-alkyl- or aryl-sulfonic acids which are unsubstituted or substituted (for example, by a halogen) such as methane- or p-toluene

sulfonic acid. Suitable hydroxides include inorganic hydroxides, such as sodium hydroxide, potassium hydroxide, calcium hydroxide, aluminium hydroxide. Alcohols include alkanealcohols of 1-12 carbon atoms which may be unsubstituted or substituted, e.g. by a halogen).

5

ENANTIOMERS/TAUTOMERS

In all aspects of the present invention previously discussed, the invention includes, where appropriate all enantiomers and tautomers of the PLK modulators or candidate compounds of the invention. The man skilled in the art will recognise compounds that
10 possess an optical properties (one or more chiral carbon atoms) or tautomeric characteristics. The corresponding enantiomers and/or tautomers may be isolated/prepared by methods known in the art.

STEREO AND GEOMETRIC ISOMERS

15 Some of the PLK modulators or candidate compounds of the invention may exist as stereoisomers and/or geometric isomers, e.g. they may possess one or more asymmetric and/or geometric centres and so may exist in two or more stereoisomeric and/or geometric forms. The present invention contemplates the use of all the individual stereoisomers and geometric isomers of those agents, and mixtures thereof. The terms
20 used in the claims encompass these forms, provided said forms retain the appropriate functional activity (though not necessarily to the same degree).

The present invention also includes all suitable isotopic variations of the PLK modulators or candidate compounds, or pharmaceutically acceptable salts thereof. An
25 isotopic variation of a PLK modulator or candidate compound of the present invention or a pharmaceutically acceptable salt thereof is defined as one in which at least one atom is replaced by an atom having the same atomic number but an atomic mass different from the atomic mass usually found in nature. Examples of isotopes that can be incorporated into the agent and pharmaceutically acceptable salts thereof include
30 isotopes of hydrogen, carbon, nitrogen, oxygen, phosphorus, sulphur, fluorine and chlorine such as ^{2}H, ^{3}H, ^{13}C, ^{14}C, ^{15}N, ^{17}O, ^{18}O, ^{31}P, ^{32}P, ^{35}S, ^{18}F and ^{36}Cl, respectively. Certain isotopic variations of the agent and pharmaceutically acceptable salts thereof,

for example, those in which a radioactive isotope such as ^{3}H or ^{14}C is incorporated, are useful in drug and/or substrate tissue distribution studies. Tritiated, i.e., ^{3}H, and carbon-14, i.e., ^{14}C, isotopes are particularly preferred for their ease of preparation and detectability. Further, substitution with isotopes such as deuterium, i.e., ^{2}H, may afford certain therapeutic advantages resulting from greater metabolic stability, for example, increased *in vivo* half-life or reduced dosage requirements and hence may be preferred in some circumstances. Isotopic variations of the PLK modulators or candidate compounds of the present invention can generally be prepared by conventional procedures using appropriate isotopic variations of suitable reagents.

SOLVATES

The present invention also includes solvate forms of the PLK modulators or candidate compounds, for example, hydrates. The terms used in the claims encompass these forms.

POLYMORPHS

The invention furthermore relates to PLK modulators or candidate compounds of the present invention in their various crystalline forms, polymorphic forms and (an)hydrous forms. It is well established within the pharmaceutical industry that chemical compounds may be isolated in any of such forms by slightly varying the method of purification and or isolation form the solvents used in the synthetic preparation of such compounds.

PRODRUGS

The invention further includes PLK modulators or candidate compounds of the present invention in prodrug form. Such prodrugs are generally compounds of the invention wherein one or more appropriate groups have been modified such that the modification may be reversed upon administration to a human or mammalian subject. Such reversion is usually performed by an enzyme naturally present in such subject, though it is possible for a second agent to be administered together with such a prodrug in order to perform the reversion in vivo. Examples of such modifications include ester (for

example, any of those described above), wherein the reversion may be carried out be an esterase etc. Other such systems will be well known to those skilled in the art.

THERAPEUTIC USE

The PLK modulators or candidate compounds of the present invention have been found to possess anti-proliferative activity and are therefore believed to be of use in the treatment of proliferative disorders, such as cancers, leukaemias or other disorders associated with uncontrolled cellular proliferation such as psoriasis and restenosis.

A further aspect of the invention therefore relates to a method of treating a proliferative disorder, said method comprising administering to a subject in need thereof a compound selected from the following:

(i) 5'-thioadenosine, or a derivative thereof;

(ii) staurosporine, wortmannin, purvalanol A, LY294002, quercetin, morin hydrate or derivatives thereof; and

(iii) 4-[4-(4-methyl-2-methylaminothiazol-5-yl)-pyrimidin-2-ylamino]-phenol, 4-[4-(2,4-dimethylthiazol-5-yl)-pyrimidin-2-ylamino]-phenol or 4-[4-(2-amino-4-methyl thiazol-5-yl)-pyrimidin-2-ylamino]-phenol;

or a pharmaceutically acceptable salt thereof, in an amount sufficient to inhibit PLK such that said proliferative disorder is treated.

Another aspect relates to a method of treating a proliferative disorder comprising inhibiting PLK by administering to a subject in need thereof, a therapeutically effective amount of a compound selected from the following:

(i) 5'-thioadenosine, or a derivative thereof;

(ii) staurosporine, wortmannin, purvalanol A, LY294002, quercetin, morin hydrate or derivatives thereof; and

(iii) 4-[4-(4-methyl-2-methylaminothiazol-5-yl)-pyrimidin-2-ylamino]-phenol, 4-[4-(2,4-dimethyl-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol or 4-[4-(2-amino-4-methyl-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol;

or a pharmaceutically acceptable salt thereof, such that treatment of the proliferative disorder occurs.

Another aspect of the invention relates to a method of preventing and/or treating a PLK related disorder comprising administering a PLK modulator or candidate compound of the invention and/or a pharmaceutical composition according to the invention, wherein said PLK modulator, said candidate compound or said pharmaceutical, is capable of causing a beneficial preventative and/or therapeutic effect.

Preferably, for this aspect, the PLK modulator or candidate compound is selected from the following:

(i) 5'-thioadenosine, or a derivative thereof:

(ii) staurosporine, wortmannin, purvalanol A, LY294002, quercetin, morin hydrate, or derivatives thereof; and

(iii) 4-[4-(4-methyl-2-methylaminothiazol-5-yl)-pyrimidin-2-ylamino]-phenol, 4-[4-(2,4-dimethyl-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol or 4-[4-(2-amino-4-methyl-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol;

or a pharmaceutically acceptable salt thereof.

A further aspect of the invention relates to the use of a PLK modulator or candidate compound according to the invention in the preparation of a medicament for treating a PLK related disorder. Preferably, the PLK related disorder is a proliferative disorder, more preferably cancer.

As used herein the phrase "preparation of a medicament" includes the use of the compound directly as the medicament in addition to its use in a screening programme for further therapeutic agents or in any stage of the manufacture of such a medicament.

Another aspect relates to a method of treating a PLK dependent disorder in a subject in need thereof, said method comprising administering to said subject a compound selected from the following:

(i) 5'-thioadenosine, or a derivative thereof;

(ii) staurosporine, wortmannin, purvalanol A, LY294002, quercetin, morin hydrate, or derivatives thereof; and

(iii) 4-[4-(4-methyl-2-methylaminothiazol-5-yl)-pyrimidin-2-ylamino]-phenol, 4-[4-(2,4-dimethyl-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol or 4-[4-(2-amino-4-methyl-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol;

or a pharmaceutically acceptable salt thereof, in an amount sufficient to inhibit PLK.

Preferably, the PLK dependent disorder is a disorder associated with increased PLK activity. Even more preferably, the disorder is cancer.

The term "proliferative disorder" is used herein in a broad sense to include any disorder that requires control of the cell cycle, for example cardiovascular disorders such as restenosis and cardiomyopathy, auto-immune disorders such as glomerulonephritis and rheumatoid arthritis, dermatological disorders such as psoriasis, anti-inflammatory, anti-fungal, antiparasitic disorders such as malaria, emphysema and alopecia. In these disorders, the compounds of the present invention may induce apoptosis or maintain stasis within the desired cells as required.

Preferably, the proliferative disorder is a cancer or leukaemia.

In another preferred embodiment, the proliferative disorder is psoriasis.

The compounds of the invention may inhibit any of the steps or stages in the cell cycle, for example, formation of the nuclear envelope, exit from the quiescent phase of the cell cycle (G0), G1 progression, chromosome decondensation, nuclear envelope breakdown, START, initiation of DNA replication, progression of DNA replication, termination of DNA replication, centrosome duplication, G2 progression, activation of mitotic or meiotic functions, chromosome condensation, centrosome separation, microtubule nucleation, spindle formation and function, interactions with microtubule motor proteins, chromatid separation and segregation, inactivation of mitotic functions, formation of contractile ring, and cytokinesis functions. In particular, the compounds of the invention may influence certain gene functions such as chromatin binding, formation of replication complexes, replication licensing, phosphorylation or other secondary modification activity, proteolytic degradation, microtubule binding, actin

binding, septin binding, microtubule organising centre nucleation activity and binding to components of cell cycle signalling pathways.

As defined herein, an anti-proliferative effect within the scope of the present invention may be demonstrated by the ability to inhibit cell proliferation in an *in vitro* whole cell assay, for example using any of the cell lines A549, HeLa, HT-29, MCF7, Saos-2, CCRF-CEM, HL-60 and K-562, or by showing kinase inhibition in an appropriate assay. These assays, including methods for their performance, are described in more detail in the accompanying Examples. Using such assays it may be determined whether a compound is anti-proliferative in the context of the present invention.

In one preferred embodiment, the compound of the invention is administered orally.

In one embodiment of the invention, the compound of the invention is administered in an amount sufficient to inhibit at least one PLK enzyme.

In a more preferred embodiment of the invention, the compound of the invention is administered in an amount sufficient to inhibit PLK1.

In one particularly preferred embodiment, the compounds of the invention are ATP-antagonistic inhibitors of PLK1.

In the present context ATP antagonism refers to the ability of an inhibitor compound to diminish or prevent PLK catalytic activity, i.e. phosphotransfer from ATP to a macromolecular PLK substrate, by virtue of reversibly or irreversibly binding at the enzyme's active site in such a manner as to impair or abolish ATP binding.

In another preferred embodiment, the compound of the invention is administered in an amount sufficient to inhibit PLK2 and/or PLK3.

Yet another aspect relates to a method of inhibiting PLK in a cell comprising contacting said cell with an amount of a compound selected from the following:

(i) 5'-thioadenosine, or a derivative thereof;

(ii) staurosporine, wortmannin, purvalanol A, LY294002, quercetin, morin hydrate, or derivatives thereof; and

(iii) 4-[4-(4-methyl-2-methylaminothiazol-5-yl)-pyrimidin-2-ylamino]-phenol, 4-[4-(2,4-dimethyl-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol or 4-[4-(2-amino-4-methyl thiazol-5-yl)-pyrimidin-2-ylamino]-phenol;

or a pharmaceutically acceptable salt thereof, such that PLK is inhibited in said cell.

Preferably, the cell is a cancer cell.

ADMINISTRATION

The pharmaceutical compositions of the present invention may be adapted for oral, rectal, vaginal, parenteral, intramuscular, intraperitoneal, intraarterial, intrathecal, intrabronchial, subcutaneous, intradermal, intravenous, nasal, buccal or sublingual routes of administration.

For oral administration, particular use is made of compressed tablets, pills, tablets, gellules, drops, and capsules. Preferably, these compositions contain from 1 to 250 mg and more preferably from 10-100 mg, of active ingredient per dose.

Other forms of administration comprise solutions or emulsions which may be injected intravenously, intraarterially, intrathecally, subcutaneously, intradermally, intraperitoneally or intramuscularly, and which are prepared from sterile or sterilisable solutions. The pharmaceutical compositions of the present invention may also be in form of suppositories, pessaries, suspensions, emulsions, lotions, ointments, creams, gels, sprays, solutions or dusting powders.

An alternative means of transdermal administration is by use of a skin patch. For example, the active ingredient can be incorporated into a cream consisting of an aqueous emulsion of polyethylene glycols or liquid paraffin. The active ingredient can also be incorporated, at a concentration of between 1 and 10% by weight, into an

ointment consisting of a white wax or white soft paraffin base together with such stabilisers and preservatives as may be required.

Injectable forms may contain between 10 - 1000 mg, preferably between 10 - 250 mg, of active ingredient per dose.

Compositions may be formulated in unit dosage form, i.e., in the form of discrete portions containing a unit dose, or a multiple or sub-unit of a unit dose.

DOSAGE

A person of ordinary skill in the art can easily determine an appropriate dose of one of the instant compositions to administer to a subject without undue experimentation. Typically, a physician will determine the actual dosage which will be most suitable for an individual patient and it will depend on a variety of factors including the activity of the specific compound employed, the metabolic stability and length of action of that compound, the age, body weight, general health, sex, diet, mode and time of administration, rate of excretion, drug combination, the severity of the particular condition, and the individual undergoing therapy. The dosages disclosed herein are exemplary of the average case. There can of course be individual instances where higher or lower dosage ranges are merited, and such are within the scope of this invention.

Depending upon the need, the agent may be administered at a dose of from 0.01 to 30 mg/kg body weight, such as from 0.1 to 10 mg/kg, more preferably from 0.1 to 1 mg/kg body weight.

In an exemplary embodiment, one or more doses of 10 to 150 mg/day will be administered to the patient for the treatment of malignancy.

PLK FRAGMENT

Another aspect of the invention relates to a fragment of PLK, or a homologue, mutant, or derivative thereof, comprising a ligand binding domain, said ligand binding domain

being defined by the amino acid residue structural coordinates selected from one or more of the following: L59, G60, A65, C67, A80, K82, L130, E131, C133, R135, F183 and D194.

As used herein, the term "ligand binding domain (LBD)" means the ligand binding region of PLK which is responsible for ligand binding. The term "ligand binding domain" also includes a homologue of the ligand binding domain, or a portion thereof.

As used herein, the term "portion thereof" means the structural co-ordinates corresponding to a sufficient number of amino acid residues of the PLK sequence (or homologue thereof) that are capable of interacting with a candidate compound capable of binding to the LBD. This term includes ligand binding domain amino acid residues having amino acid residues from about 4Å to about 5Å of a bound compound or fragment thereof. Thus, for example, the structural co-ordinates provided in the homology model may contain a subset of the amino acid residues in the LBD which may be useful in the modelling and design of compounds that bind to the LBD.

In one preferred embodiment, the fragment of PLK, or a homologue, mutant or derivative thereof, corresponds to a portion of the structure co-ordinates of *Table 2*.

Another aspect of the invention relates to the use of the above-described fragment of PLK, or a homologue, mutant, or derivative thereof, in an assay for identifying candidate compounds capable of modulating PLK.

The PLK proteins produced by a host recombinant cell may be secreted or may be contained intracellularly depending on the nucleotide sequence and/or the vector used.

As will be understood by those skilled in the art, expression vectors containing a PLK encoding nucleotide sequence or a mutant, variant, homologue, derivative or fragment thereof, may be designed with signal sequences which direct secretion of the PLK coding sequences through a particular prokaryotic or eukaryotic cell membrane.

The PLK encoding sequence may be fused (eg. ligated) to nucleotide sequences encoding a polypeptide domain which will facilitate purification of soluble proteins (Kroll *DJ et al* (1993) DNA Cell Biol 12:441-53). Preferably, the polypeptide domain which facilitates purification of soluble proteins is fused in frame with the PLK encoding sequence. Such purification facilitating domains include, but are not limited to, metal chelating peptides – such as histidine-tryptophan modules that allow purification on immobilised metals (Porath J (1992) Protein Expr Purif 3, 263-281), protein A domains that allow purification on immobilised immunoglobulin, and the domain utilised in the FLAGS extension/affinity purification system (Immunex Corp, Seattle, WA). The inclusion of a cleavable linker sequence such as Factor XA or enterokinase (Invitrogen, San Diego, CA) between the purification domain and PLK is useful to facilitate purification.

NUCLEOTIDE SEQUENCES

As used herein, the term "nucleotide sequence" refers to nucleotide sequences, oligonucleotide sequences, polynucleotide sequences and variants, homologues, fragments and derivatives thereof (such as portions thereof) which comprise the nucleotide sequences encoding PLK.

The nucleotide sequence may be DNA or RNA of genomic or synthetic or recombinant origin, which may be double-stranded or single-stranded whether representing the sense or antisense strand or combinations thereof.

Preferably, the term nucleotide sequence is prepared by use of recombinant DNA techniques (e.g. recombinant DNA). The nucleotide sequences may include within them synthetic or modified nucleotides. A number of different types of modification to oligonucleotides are known in the art. These include methylphosphonate and phosphorothioate backbones, addition of acridine or polylysine chains at the 3' and/or 5' ends of the molecule. For the purposes of the present invention, it is to be understood that the nucleotide sequences described herein may be modified by any method available in the art.

It will be understood by a skilled person that numerous different nucleotide sequences can encode the same protein as a result of the degeneracy of the genetic code. In addition, it is to be understood that skilled persons may, using routine techniques, make nucleotide substitutions that do not substantially affect the activity encoded by the nucleotide sequence of the present invention to reflect the codon usage of any particular host organism in which the target is to be expressed. Thus, the terms "variant", "homologue" or "derivative" in relation to nucleotide sequences include any substitution of, variation of, modification of, replacement of, deletion of or addition of one (or more) nucleic acids from or to the sequence providing the resultant nucleotide sequence encodes a functional protein according to the present invention (or even a modulator of PLK according to the present invention if said modulator comprises a nucleotide sequence or an amino acid sequence).

AMINO ACID SEQUENCES

As used herein, the term "amino acid sequence" is synonymous with the term "polypeptide" and/or the term "protein". In some instances, the term "amino acid sequence" is synonymous with the term "peptide".

The amino acid sequence may be isolated from a suitable source, or it may be made synthetically or it may be prepared by use of recombinant DNA techniques.

VARIANTS/HOMOLOGUES/DERIVATIVES/FRAGMENTS

The PLK described herein is intended to include any polypeptide, which has the activity of the naturally occurring PLK and includes all vertebrate and mammalian forms. Such terms also include polypeptides that differ from naturally occurring forms of PLK by having amino acid deletions, substitutions, and additions, but which retain the activity of PLK.

The term "variant" is used to mean a naturally occurring polypeptide or nucleotide sequences which differs from a wild-type or a native sequence.

The term "fragment" indicates that a polypeptide or nucleotide sequence comprises a fraction of a wild-type or a native sequence. It may comprise one or more large contiguous sections of sequence or a plurality of small sections. The sequence may also comprise other elements of sequence, for example, it may be a fusion protein with another protein. Preferably the sequence comprises at least 50%, more preferably at least 65%, more preferably at least 80%, most preferably at least 90% of the wild-type sequence.

The present invention also encompasses the use of variants, homologues and derivatives of nucleotide and amino acid sequences. Here, the term "homologue" means an entity having a certain homology with amino acid sequences or nucleotide sequences. Here, the term "homology" can be equated with "identity".

In the present context, an homologous sequence is taken to include an amino acid sequence which may be at least 75, 85 or 90% identical, preferably at least 95 or 98% identical to the subject sequence. Although homology can also be considered in terms of similarity (i.e. amino acid residues having similar chemical properties/functions), it is preferred to express homology in terms of sequence identity.

An homologous sequence is taken to include a nucleotide sequence which may be at least 75, 85 or 90% identical, preferably at least 95 or 98% identical to the subject sequence.

Homology comparisons can be conducted by eye, or more usually, with the aid of readily available sequence comparison programs. These commercially available computer programs can calculate % homology between two or more sequences.

% homology may be calculated over contiguous sequences, i.e. one sequence is aligned with the other sequence and each amino acid in one sequence is directly compared with the corresponding amino acid in the other sequence, one residue at a time. This is called an "ungapped" alignment. Typically, such ungapped alignments are performed only over a relatively short number of residues.

Although this is a very simple and consistent method, it fails to take into consideration that, for example, in an otherwise identical pair of sequences, one insertion or deletion will cause the following amino acid residues to be put out of alignment, thus potentially resulting in a large reduction in % homology when a global alignment is performed. Consequently, most sequence comparison methods are designed to produce optimal alignments that take into consideration possible insertions and deletions without penalising unduly the overall homology score. This is achieved by inserting "gaps" in the sequence alignment to try to maximise local homology.

However, these more complex methods assign "gap penalties" to each gap that occurs in the alignment so that, for the same number of identical amino acids, a sequence alignment with as few gaps as possible - reflecting higher relatedness between the two compared sequences - will achieve a higher score than one with many gaps. "Affine gap costs" are typically used that charge a relatively high cost for the existence of a gap and a smaller penalty for each subsequent residue in the gap. This is the most commonly used gap scoring system. High gap penalties will of course produce optimised alignments with fewer gaps. Most alignment programs allow the gap penalties to be modified. However, it is preferred to use the default values when using such software for sequence comparisons. For example when using the GCG Wisconsin Bestfit package the default gap penalty for amino acid sequences is -12 for a gap and -4 for each extension.

Calculation of maximum % homology therefore firstly requires the production of an optimal alignment, taking into consideration gap penalties. A suitable computer program for carrying out such an alignment is the GCG Wisconsin Bestfit package (University of Wisconsin, U.S.A.; Devereux *et al.*, 1984, Nucleic Acids Research 12:387). Examples of other software than can perform sequence comparisons include, but are not limited to, the BLAST package (see Ausubel *et al.*, 1999 ibid – Chapter 18), FASTA (Atschul *et al.*, 1990, J. Mol. Biol., 403-410) and the GENEWORKS suite of comparison tools. Both BLAST and FASTA are available for offline and online searching (see Ausubel *et al.*, 1999 ibid, pages 7-58 to 7-60). However, for some applications, it is preferred to use the GCG Bestfit program. A new tool, called BLAST

2 Sequences is also available for comparing protein and nucleotide sequence (see *FEMS Microbiol Lett* 1999 174(2): 247-50; *FEMS Microbiol Lett* 1999 177(1): 187-8)

Although the final % homology can be measured in terms of identity, the alignment process itself is typically not based on an all-or-nothing pair comparison. Instead, a scaled similarity score matrix is generally used that assigns scores to each pairwise comparison based on chemical similarity or evolutionary distance. An example of such a matrix commonly used is the BLOSUM62 matrix - the default matrix for the BLAST suite of programs. GCG Wisconsin programs generally use either the public default values or a custom symbol comparison table if supplied (see user manual for further details). For some applications, it is preferred to use the public default values for the GCG package, or in the case of other software, the default matrix, such as BLOSUM62. Once the software has produced an optimal alignment, it is possible to calculate % homology, preferably % sequence identity. The software typically does this as part of the sequence comparison and generates a numerical result.

The sequences may also have deletions, insertions or substitutions of amino acid residues, which produce a silent change and result in a functionally equivalent substance. Deliberate amino acid substitutions may be made on the basis of similarity in polarity, charge, solubility, hydrophobicity, hydrophilicity, and/or the amphipathic nature of the residues as long as the secondary binding activity of the substance is retained. For example, negatively charged amino acids include aspartic acid and glutamic acid; positively charged amino acids include lysine and arginine; and amino acids with uncharged polar head groups having similar hydrophilicity values include leucine, isoleucine, valine, glycine, alanine, asparagine, glutamine, serine, threonine, phenylalanine, and tyrosine.

Conservative substitutions may be made, for example according to the Table below. Amino acids in the same block in the second column and preferably in the same line in the third column may be substituted for each other:

ALIPHATIC	Non-polar	G A P
		I L V
	Polar - uncharged	C S T M
		N Q
	Polar - charged	D E
		K R
AROMATIC		H F W Y

Homologous substitution (substitution and replacement are both used herein to mean the interchange of an existing amino acid residue, with an alternative residue) may occur i.e. like-for-like substitution such as basic for basic, acidic for acidic, polar for polar etc. Non-homologous substitution may also occur i.e. from one class of residue to another or alternatively involving the inclusion of unnatural amino acids such as ornithine (hereinafter referred to as Z), diaminobutyric acid ornithine (hereinafter referred to as B), norleucine ornithine (hereinafter referred to as O), pyriylalanine, thienylalanine, naphthylalanine and phenylglycine.

Replacements may also be made by unnatural amino acids include; alpha* and alpha-disubstituted* amino acids, N-alkyl amino acids*, lactic acid*, halide derivatives of natural amino acids such as trifluorotyrosine*, p-Cl-phenylalanine*, p-Br-phenylalanine*, p-I-phenylalanine*, L-allyl-glycine*, ß-alanine*, L-α-amino butyric acid*, L-γ-amino butyric acid*, L-α-amino isobutyric acid*, L-ε-amino caproic acid#, 7-amino heptanoic acid*, L-methionine sulfone#*, L-norleucine*, L-norvaline*, p-nitro-L-phenylalanine*, L-hydroxyproline#, L-thioproline*, methyl derivatives of phenylalanine (Phe) such as 4-methyl-Phe*, pentamethyl-Phe*, L-Phe (4-amino)#, L-Tyr (methyl)*, L-Phe (4-isopropyl)*, L-Tic (1,2,3,4-tetrahydroisoquinoline-3-carboxyl acid)*, L-diaminopropionic acid # and L-Phe (4-benzyl)*. The notation * has been utilised for the purpose of the discussion above (relating to homologous or non-homologous substitution), to indicate the hydrophobic nature of the derivative whereas # has been utilised to indicate the hydrophilic nature of the derivative, #* indicates amphipathic characteristics.

The term "derivative" or "derivatised" as used herein includes chemical modification of an entity, such as candidate compound or a PLK modulator. Illustrative of such chemical modifications would be replacement of hydrogen by a halo group, an alkyl group, an acyl group or an amino group.

Variant amino acid sequences may include suitable spacer groups that may be inserted between any two amino acid residues of the sequence including alkyl groups such as methyl, ethyl or propyl groups in addition to amino acid spacers such as glycine or β-alanine residues. A further form of variation, involves the presence of one or more amino acid residues in peptoid form, will be well understood by those skilled in the art. For the avoidance of doubt, "the peptoid form" is used to refer to variant amino acid residues wherein the α-carbon substituent group is on the residue's nitrogen atom rather than the α-carbon. Processes for preparing peptides in the peptoid form are known in the art, for example Simon RJ et al., PNAS (1992) 89(20), 9367-9371 and Horwell DC, Trends Biotechnol. (1995) 13(4), 132-134.

MUTANT

As used herein, the term "mutant" refers to PLK comprising one or more changes in the wild-type PLK sequence.

The term "mutant" is not limited to amino acid substitutions of the amino acid residues in PLK, but also includes deletions or insertions of nucleotides which may result in changes in the amino acid residues in the amino acid sequence of PLK.

The present invention also enables the solving of the crystal structure of PLK mutants. More particularly, by virtue of the present invention, the location of the active site of PLK based on the structural coordinates of *Table 2* permits the identification of desirable sites for mutation. For example, one or more mutations may be directed to a particular site - such as the active site - or combination of sites of PLK. Similarly, only a location on, at or near the enzyme surface may be replaced, resulting in an altered surface charge of one or more charge units, as compared to the wild-type enzyme. Alternatively, an amino acid

residue in PLK may be chosen for replacement based on its hydrophilic or hydrophobic characteristics.

Such mutants may be characterised by any one of several different properties as compared with wild-type PLK. For example, such mutants may have altered surface charge of one or more charge units, or have an increased stability to subunit dissociation, or an altered substrate specificity in comparison with, or a higher specific activity than, wild-type PLK.

The mutants may be prepared in a number of ways that are known by a person skilled in the art. For example, mutations may be introduced by means of oligonucleotide-directed mutagenesis or other conventional methods. Alternatively, mutants of PLK may be generated by site specific replacement of a particular amino acid with an unnaturally occurring amino acid. This may be achieved by growing a host organism capable of expressing either the wild-type or mutant polypeptide on a growth medium depleted of one or more natural amino acids but enriched in one or more corresponding unnaturally occurring amino acids.

HOST CELLS

As used herein, the term "host cell" refers to any cell that comprises nucleotide sequences that are of use in the present invention, for example, nucleotide sequences encoding PLK.

Host cells may be transformed or transfected with a nucleotide sequence contained in a vector e.g. a cloning vector. Preferably, said nucleotide sequence is carried in a vector for the replication and/or expression of the nucleotide sequence. The cells will be chosen to be compatible with the said vector and may for example be prokaryotic (for example bacterial), fungal, yeast or plant cells.

The gram-negative bacterium *E. coli* is widely used as a host for cloning nucleotide sequences. This organism is also widely used for heterologous nucleotide sequence expression. However, large amounts of heterologous protein tend to accumulate inside

the cell. Subsequent purification of the desired protein from the bulk of *E. coli* intracellular proteins can sometimes be difficult.

In contrast to *E. coli*, bacteria from the genus Bacillus are very suitable as heterologous hosts because of their capability to secrete proteins into the culture medium. Other bacteria suitable as hosts are those from the genera Streptomyces and Pseudomonas.

Depending on the nature of the polynucleotide and/or the desirability for further processing of the expressed protein, eukaryotic hosts including yeasts or other fungi may be preferred. In general, yeast cells are preferred over fungal cells because yeast cells are easier to manipulate. However, some proteins are either poorly secreted from the yeast cell, or in some cases are not processed properly (*e.g.* hyperglycosylation in yeast). In these instances, a different fungal host organism should be selected.

Examples of expression hosts are fungi - such as Aspergillus species (such as those described in EP-A-0184438 and EP-A-0284603) and Trichoderma species; bacteria - such as Bacillus species (such as those described in EP-A-0134048 and EP-A-0253455), Streptomyces species and Pseudomonas species; yeasts - such as Kluyveromyces species (such as those described in EP-A-0096430 and EP-A-0301670) and Saccharomyces species; and mammalian cells – such as CHO-K1 cells.

The use of host cells may provide for post-translational modifications as may be needed to confer optimal biological activity on recombinant expression products of the present invention.

Aspects of the present invention also relate to host cells comprising the PLK constructs of the present invention. The PLK constructs may comprise a nucleotide sequence for replication and expression of the sequence. The cells will be chosen to be compatible with the vector and may for example be prokaryotic (for example bacterial), fungal, yeast or plant cells.

In a preferred embodiment, the host cells are mammalian cells, such as CHO-K1 cells.

VECTOR

Aspects of the present invention relate to a vector comprising a nucleotide sequence, such as a nucleotide sequence encoding PLK or a modulator of PLK, administered to a subject.

Preferably, PLK or the modulator of PLK is prepared and/or delivered using a genetic vector.

As it is well known in the art, a vector is a tool that allows or facilitates the transfer of an entity from one environment to another. In accordance with the present invention, and by way of example, some vectors used in recombinant DNA techniques allow entities, such as a segment of DNA (such as a heterologous DNA segment, such as a heterologous cDNA segment), to be transferred into a host and/or a target cell for the purpose of replicating the vectors comprising nucleotide sequences and/or expressing the proteins encoded by the nucleotide sequences. Examples of vectors used in recombinant DNA techniques include, but are not limited to, plasmids, chromosomes, artificial chromosomes or viruses.

The term "vector" includes expression vectors and/or transformation vectors.

The term "expression vector" means a construct capable of *in vivo* or *in vitro/ex vivo* expression.

The term "transformation vector" means a construct capable of being transferred from one species to another.

REGULATORY SEQUENCES

In some applications, nucleotide sequences are operably linked to a regulatory sequence which is capable of providing for the expression of the nucleotide sequence, such as by a chosen host cell. By way of example, a vector comprising the PLK nucleotide sequence is operably linked to such a regulatory sequence i.e. the vector is an expression vector.

The term "operably linked" refers to a juxtaposition wherein the components described are in a relationship permitting them to function in their intended manner. A regulatory sequence "operably linked" to a coding sequence is ligated in such a way that expression of the coding sequence is achieved under conditions compatible with the control sequences.

The term "regulatory sequences" includes promoters and enhancers and other expression regulation signals.

The term "promoter" is used in the normal sense of the art, e.g. an RNA polymerase binding site.

Enhanced expression of a nucleotide sequence, for example, a nucleotide sequence encoding PLK, may also be achieved by the selection of heterologous regulatory regions, e.g. promoter, secretion leader and terminator regions, which serve to increase expression and, if desired, secretion levels of the protein of interest from the chosen expression host and/or to provide for the inducible control of the expression of PLK. In eukaryotes, polyadenylation sequences may be operably connected to the PLK nucleotide sequence.

Preferably, the PLK nucleotide sequence is operably linked to at least a promoter.

Aside from the promoter native to the gene encoding the PLK nucleotide sequence, other promoters may be used to direct expression of the PLK polypeptide. The promoter may be selected for its efficiency in directing the expression of the PLK nucleotide sequence in the desired expression host.

In another embodiment, a constitutive promoter may be selected to direct the expression of the PLK nucleotide sequence. Such an expression construct may provide additional advantages since it circumvents the need to culture the expression hosts on a medium containing an inducing substrate.

Hybrid promoters may also be used to improve inducible regulation of the expression construct.

The promoter can additionally include features to ensure or to increase expression in a suitable host. For example, the features can be conserved regions such as a Pribnow Box or a TATA box. The promoter may even contain other sequences to affect (such as to maintain, enhance, decrease) the levels of expression of the PLK nucleotide sequence. For example, suitable other sequences include the Sh1-intron or an ADH intron. Other sequences include inducible elements - such as temperature, chemical, light or stress inducible elements. Also, suitable elements to enhance transcription or translation may be present.

EXPRESSION VECTOR

Preferably, nucleotide sequences, such as nucleotide sequences encoding PLK or modulators of PLK, are inserted into a vector that is operably linked to a control sequence that is capable of providing for the expression of the coding sequence by the host cell.

Nucleotide sequences produced by a host recombinant cell may be secreted or may be contained intracellularly depending on the sequence and/or the vector used. As will be understood by those of skill in the art, expression vectors can be designed with signal sequences, which direct secretion of the nucleotide sequence through a particular prokaryotic or eukaryotic cell membrane.

Preferably, the expression vectors are stably expressed in CHO cells as described previously (Ehlers *et al.* (1996) *Biochemistry 35*, 9549-9559). More preferably, the expression vectors are pLEN- tACEΔ36g(1, 2, 3, 4) and pLEN- tACEΔ36g(1,3).

FUSION PROTEINS

PLK or a modulator of PLK may be expressed as a fusion protein to aid extraction and purification and/or delivery of the modulator of PLK or the PLK protein to an individual and/or to facilitate the development of a screen for modulators of PLK.

Examples of fusion protein partners include glutathione-S-transferase (GST), 6xHis, GAL4 (DNA binding and/or transcriptional activation domains) and β-galactosidase.

It may also be convenient to include a proteolytic cleavage site between the fusion protein partner and the protein sequence of interest to allow removal of fusion protein sequences. Preferably, the fusion protein will not hinder the activity of the protein of interest.

The fusion protein may comprise an antigen or an antigenic determinant fused to the substance of the present invention. In this embodiment, the fusion protein may be a non-naturally occurring fusion protein comprising a substance, which may act as an adjuvant in the sense of providing a generalised stimulation of the immune system. The antigen or antigenic determinant may be attached to either the amino or carboxy terminus of the substance.

ORGANISM

The term "organism" in relation to the present invention includes any organism that could comprise PLK and/or modulators of PLK. Examples of organisms may include mammals, fungi, yeast or plants.

Preferably, the organism is a mammal. More preferably, the organism is a human.

TRANSFORMATION

As indicated earlier, the host organism can be a prokaryotic or a eukaryotic organism. Examples of suitable prokaryotic hosts include *E. coli* and *Bacillus subtilis*. Teachings on the transformation of prokaryotic hosts are well documented in the art, for example see Sambrook et al (Molecular Cloning: A Laboratory Manual, 2nd edition, 1989, Cold Spring Harbor Laboratory Press) and Ausubel *et al.*, Current Protocols in Molecular Biology (1995), John Wiley & Sons, Inc. Examples of suitable eukaryotic hosts include mammalian cells.

If a prokaryotic host is used then the nucleotide sequence, such as the PLK nucleotide sequence, may need to be suitably modified before transformation - such as by removal of introns.

Thus, the present invention also relates to the transformation of a host cell with a nucleotide sequence, such as PLK or a modulator of PLK. Host cells transformed with the nucleotide sequence may be cultured under conditions suitable for the expression and recovery of the encoded protein from cell culture. The protein produced by a recombinant cell may be secreted or may be contained intracellularly depending on the sequence and/or the vector used. As will be understood by those of skill in the art, expression vectors containing coding sequences can be designed with signal sequences which direct secretion of the coding sequences through a particular prokaryotic or eukaryotic cell membrane. Other recombinant constructions may join the coding sequence to nucleotide sequence encoding a polypeptide domain, which will facilitate purification of soluble proteins (Kroll *DJ et al* (1993) DNA Cell Biol 12:441-53) e.g. 6-His or Glutathione-*S*-transferase.

TRANSFECTION

Vectors comprising for example, the PLK nucleotide sequence, may be introduced into host cells, for example, mammalian cells, using a variety of methods.

Typical transfection methods include electroporation, DNA biolistics, lipid-mediated transfection, compacted DNA-mediated transfection, liposomes, immunoliposomes, lipofectin, cationic agent-mediated, cationic facial amphiphiles (CFAs) (*Nature Biotech.* (1996) 14, 556), multivalent cations such as spermine, cationic lipids or polylysine, 1, 2,-bis (oleoyloxy)-3-(trimethylammonio) propane (DOTAP)-cholesterol complexes (Wolff and Trubetskoy 1998 Nature Biotechnology 16: 421) and combinations thereof.

Uptake of nucleic acid constructs by mammalian cells is enhanced by several known transfection techniques for example those including the use of transfection agents. Example of these agents include cationic agents (for example calcium phosphate and

DEAE-dextran) and lipofectants (for example lipofectam™ and transfectam™). Typically, nucleic acid constructs are mixed with the transfection agent to produce a composition.

Such methods are described in many standard laboratory manuals - such as Sambrook *et al.*, Molecular Cloning: A Laboratory Manual, 2d ed. (1989) Cold Spring Harbor Laboratory Press, Cold Spring Harbor, N.Y.

The present invention is further described by way of example, and with reference to the following figures wherein:

Figure 1 shows multiple sequence alignment (Clustal W) of human PLK1 (P53350), PLK2 (Q9NYY3), and PLK3 (Q9H4B4).

Figure 2 shows a schematic view of PLK1 homology model in complex with ATP (stick model, labelled). The protein structure is indicated with a ribbon (loops, thin; helices, thick; sheets, arrows). The Cys residues are shown with space-filled atoms and are labelled.

Figure 3 shows sequence alignment of PLK1 and PKA kinase domains.

Figure 4 shows modelled complex between PLK1 and ATP (a) and 5'-thioadenosine (b). The positions of the thiol groups (SH) of Cys^{67} and 5'thioadenosine are indicated.

Figure 5 shows dose response curves of PLK1 activity inhibition by various adenosine derivatives in the absence or presence of the reducing agent dithiothreitol (+DTT or –DTT).

Figure 6 shows kinetic analysis of PLK1 inhibition by 5'-thioadenosine.

Figure 7 shows modelled PLK1-bound conformations of ATP (a); 5'-thioadenosine (b); staurosporine (c); and 4-[4-(4-methyl-2-methylamino-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol (d). Non-H atoms are labelled.

Figure 8 shows dose response curves for Purvalanol A, staurosporine and wortmannin.

Figure 9 shows the ATP dependence of PLK1 inhibition by staurosporine (a) and wortmannin (b).

Figure 10 shows the Inhibition of PLK1 and Casein Kinase II by Wortmannin and LY294002.

Figure 11 shows docked structures of A) purvalanol A and B) morin hydrate with the ATP binding site of the PLK1 model structure.

Figure 12 shows modelled structure of wortmannin covalently bound to K82 in the ATP cleft of PLK1. The right panel view is rotated by 180° along the y axis relative to the left view.

Figure 13 shows a Lineweaver-Burk plot analysis of the ATP dependence of Inhibitor A.

Figure 14 shows a Lineweaver-Burk plot analysis of the ATP dependence of Inhibitor B.

Figure 15 shows the modelled structure of Inhibitor B in the binding pocket of PLK1, showing the close proximity of the potential reactive atoms of Inhibitor B to the cysteine (C67) residue of PLK1.

EXAMPLES

General Methods

The methods described here may employ, unless otherwise indicated, conventional techniques of chemistry, molecular biology, microbiology, recombinant DNA and immunology, which are within the capabilities of a person of ordinary skill in the art. Such techniques are explained in the literature. See, for example, J. Sambrook, E. F. Fritsch, and T. Maniatis, 1989, *Molecular Cloning: A Laboratory Manual*, Second Edition, Books 1-3, Cold Spring Harbor Laboratory Press; Ausubel, F. M. et al. (1995 and periodic supplements; *Current Protocols in Molecular Biology*, ch. 9, 13, and 16, John Wiley & Sons, New York, N.Y.); B. Roe, J. Crabtree, and A. Kahn, 1996, *DNA Isolation and Sequencing: Essential Techniques*, John Wiley & Sons; J. M. Polak and James O'D. McGee, 1990, *In Situ Hybridization: Principles and Practice*; Oxford University Press; M. J. Gait (Editor), 1984, *Oligonucleotide Synthesis: A Practical Approach*, Irl Press; D. M. J. Lilley and J. E. Dahlberg, 1992, *Methods of Enzymology: DNA Structure Part A: Synthesis and Physical Analysis of DNA* Methods in Enzymology, Academic Press; Using Antibodies : A Laboratory Manual : Portable Protocol NO. I by Edward Harlow, David Lane, Ed Harlow (1999, Cold Spring Harbor Laboratory Press, ISBN 0-87969-544-7); Antibodies : A Laboratory Manual by Ed Harlow (Editor), David Lane (Editor) (1988, Cold Spring Harbor Laboratory Press, ISBN 0-87969-314-2), 1855. Handbook of Drug Screening, edited by Ramakrishna Seethala, Prabhavathi B. Fernandes (2001, New York, NY, Marcel Dekker, ISBN 0-8247-0562-9); and Lab Ref: A Handbook of Recipes, Reagents, and Other Reference Tools for Use at the Bench, Edited Jane Roskams and Linda Rodgers, 2002, Cold Spring Harbor Laboratory, ISBN 0-87969-630-3. Each of these general texts is herein incorporated by reference.

Example 1

Construction of PLK1 homology model

The homology model for PLK1 kinase domain was generated using the program module Homology within the molecular modelling package Insight II (Accelrys, San Diego, CA) [38]. The sequence containing the kinase domain of PLK1 (residues 1 –

356) was employed in a FASTA sequence and structural search [39] in order to find the closest sequence-related kinase for which experimental structural information was available. For this search, the BLOSUM 50 scoring matrix [40] and a specific residue string value of 2 was employed. The closest match of known structure proved to be that of cAMP-dependent protein kinase (protein kinase A, PKA) with a sequence identity of 30 % and similarity of close to 50 % (*Figure 3*). Although these values are typically low for homology model building, the structural conservation of protein kinases was thought to allow a valid structure to be generated. Sequence alignment of PLK1 kinase domain with PKA in addition to CDK2 and ERK2 (which also were among the most homologous structures) indicated that the minimal kinase domain included residues 52 – 308. For the sequence alignment, the PAM 120 multiple scoring matrix [41] was used with a dimension block of 0.6, a high significance p value of 0.0001, a not significant p value of 0.1, and a pair-wise threshold of 60. Using a combination of the three structures to generate coordinates for the regions that had the highest identity in each kinase (*Table 1*), a model structure for the kinase domain was constructed. The strategy generally involved using PKA to define the structurally conserved regions (SCRs) from which the coordinates were subsequently transferred. This was then followed by loop construction where the non-SCRs were generated by *de-novo* building and subsequent evaluation of the most realistic coordinates (in terms of energetics of the loop itself and the exclusion of loops leading to overlapping atoms). After loop building was completed for missing coordinates, the raw coordinates were then refined using successive rounds of end repair splice repairing using an omega force constant of 50, energy minimization (100 steps of steepest descent to a derivative of 5). The model was then completed through using a further minimisation and 1 ps of molecular dynamics to more fully explore the conformational space of the loop regions. The final model structure was then checked against databases of protein structures for bond length and dihedral angle violations. The results indicated that these as a whole were within acceptable limits with > 80 % of residues having phi-psi plots with the allowed region in Ramachandran space [42]. The coordinate file for the final PLK1 homology model – ATP complex in Brookhaven Protein Databank (PDB) format [43] is shown in *Table 2*.

Example 2

Production of recombinant human PLK1

The human PLK1 (SwissProt accession number P53350, [44]) open reading frame (ORF) was amplified by PCR from a human foetal lung cDNA library (Clontech). An Nhe I restriction endonuclease site was introduced upstream of the ORF, by inclusion in the sense PCR primer. An Eco RI restriction endonuclease site was introduced downstream of the ORF, by inclusion in the antisense PCR primer. The PCR product generated was cloned into pCR4-Topo (Invitrogen), and sequenced. The ORF was then sub-cloned as an Nhe I / Eco RI fragment into pSSP1, a derivative of bacmid transfer vector pFastBac HTa (Invitrogen). The PLK1 ORF was cloned into pSSP1 such that the resulting PLK1 translation product would have a 19 amino acid N-terminal tag (MSYYHHHHHHGMASDDDDK) containing a hexahistidine tag and an enterokinase cleavage site. The pSSP1-Plk1 expression cassette was transferred into bacmid DNA by transposition in E. coli DH10Bac (Invitrogen). Purified recombinant bacmid DNA was transfected into Sf9 cells, to produce an infective stock of recombinant baculovirus. Following subsequent amplification and titering of the baculoviral stock, this was used to infect Sf9 cells at a multiplicity of infection of approximately 3. His-tagged PLK1 was expressed by incubating the infected cells at 27 °C, with shaking. Two days after infection, the cells were collected by centrifugation. Prior to purification, PLK1 expression was confirmed by Western blotting. To the cell pellet from 150 mL Sf9 insect cell culture 10 mL lysis buffer [10 mM Tris-HCl pH 8.0, 150 ml NaCl, 20 mM β-mercaptoethanol, 1 mM PMSF, 1 mM benzamidine, protease inhibitor cocktail (Sigma; 1 : 1,000 diluted), 20 mM imidazole], supplemented with 2 mM NaF and 1 mM Na_3VO_4, was added; the mixture was sonicated (6 × 20 s) on ice and centrifuged for 15 min at 15,000 r.p.m. The supernatant was filtered (0.45 μm filter) and the filtrate was applied to a pre-equilibrated (with 20 mL lysis buffer) 1.2-mL Ni-NTA agarose column (Qiagen). After incubation for 2 h at 4 °C, the non-bound fraction was eluted with was buffer (as lysis buffer but 300 mM NaCl and without imidazole). Protein was eluted with elution buffer (as lysis buffer but 100 mM NaCl, 250 mM imidazole, 0.02 % Nonidet P-40). Pooled fractions containing target protein were applied to an equilibrated (with dialysis buffer) 5-mL HiTrap™ desalting column (Amersham Biosciences) and eluted with dialysis buffer (25 mM Tris/MES pH 7.6, 1 mM β-

mercaptoethanol, 0.01 % Tween-20, 10 mM $MgCl_2$, 50 μM ATP, 100 mM NaCl, 1 mM PMSF, 1 mM benzamidine, 10 % glycerol). Pooled fractions containing pure target protein were centrifuged 15,000 r.p.m. for 15 min. The supernatant PLK1 stock solution was stored at –70 °C.

Example 3

Construction, expression and purification of a Cdc25C fragment

Using standard techniques, a full-length Cdc25C clone was isolated by PCR from HeLa mRNA and inserted on a *BamHI-Hind*III fragment into pRsetA. The amino terminal Cdc25C fragment (encoding residues 1-300) was excised from this vector and inserted into pET28a (between the *Nco*I and *Bam*HI sites). Expression was under the control of the T7 promoter, and the encoded protein contains a His_6 tag at the carboxy terminus. The vector was transformed into *E. coli* strain BRL(DE3) pLysS for expression experiments. The protein was expressed in BL21(DE3) RIL bacteria cells, grown in LB media at 37 °C until optical density at 600 nm of 0.6 was reached. The expression was induced with 1 mM IPTG and the bacterial culture was grown further for 3 h. The bacteria were harvested by centrifugation and the cell pellet was re-suspended in 50mM Tris pH 7.5 and 10 % sucrose, snap-frozen, and stored at –70 °C until used.

Purification of the protein was then carried out by lysing the bacterial pellet in 10 mL of lysis buffer (10mM Tris-HCl, pH 8.0, 150 mM NaCl, 5 mM β-mercaptoethanol, and 20 mM imidazole) supplemented with a cocktail of protease inhibitors, sonicated 6 times at 20-s bursts. The lysate was then centrifuged for 15 min at 15,000 r.p.m. and filtered through a 0.45-μm filter. The sample was then loaded onto a Ni-NTA agarose column, washed several times then the Cdc25C protein fragment was eluted with a buffer containing 10 mM Tris-HCl, pH 8.0, 100 mM NaCl, 5 mM β-mercaptoethanol, 0.02 % Nonidet P-40, and 250 mM imidazol. The eluate was then dialysed, concentrated, snap-frozen in liquid nitrogen, and stored at –70 °C until used.

Example 4

PLK1 assay

PLK1 kinase activity was assayed using human CDC25C phosphatase as a substrate [4]. The assays were carried out using 96-well microtitre plates by incubating CDC25C (2 μg/well) with 1 μg/well of purified human recombinant PLK1 and varying concentrations of the candidate compound in a total volume of 25 μL of 20 mM Tris/HCl buffer pH 7.5, supplemented with 25 mM β-glycerophosphate, 5 mM EGTA, 1 mM DTT, and 1 mM $NaVO_3$. Reaction was initiated by the addition of 100 μM ATP and 0.5 μCi of [γ-^{32}P]-ATP. The reaction mixture was incubated at 30 °C for 1 h, then stopped with 75 mM aq orthophosphoric acid, transferred onto a 96-well P81 filter plate (Whatman), dried, and the extent of CDC25C phosphorylation was assessed by scintillation counting using a Packard TopCount plate reader.

Example 5

Casein kinase II (CKII) assay

Human recombinant CKII activity was assayed using the peptide H-Arg-Arg-Arg-Glu-Glu-Glu-Thr-Glu-Glu-Glu-OH as a substrate. The assays were carried out using 96-well microtitre plates by incubating the peptide substrate (10 μM) with 20 Units/well of CKII (New England Biolabs) and varying concentrations of the candidate compound in a total volume of 25 μL of 25 mM MOPS buffer pH 7.0, supplemented with 25 mM β-glycerophosphate, 5 mM EGTA, 1 mM DTT, and 1 mM $NaVO_3$. Reaction was initiated by the addition of 100 μM ATP and 0.25 μCi of [γ-^{32}P]-ATP. The reaction mixture was incubated at 30 °C for 15 minutes, then stopped with 75 mM aq orthophosphoric acid, transferred onto a 96-well P81 filter plate (Whatman), dried, and the extent of peptide phosphorylation was assessed by scintillation counting using a Packard TopCount plate reader.

Example 6

Chemical kinase inhibitors

Wortmannin and LY294002 were acquired from CN Biosciences Ltd., UK. Staurosporine, quercetin, and myricetin were from Sigma Chemicals, UK. All other

flavonoid compounds were purchased from Indofine Chemical Company, Inc., Somerville, New Jersey, USA.

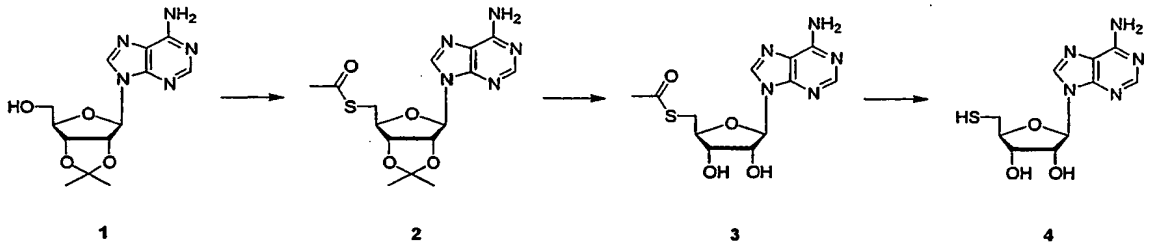
Example 7

Synthesis of Compounds

4-[4-(4-methyl-2-methylaminothiazol-5-yl)-pyrimidin-2-ylamino]-phenol, 4-[4-(2,4-dimethyl-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol and 4-[4-(2-amino-4-methyl-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol were synthesised in accordance with the methodology described in WO 01/72745. Staurosporine and derivatives thereof (such as CGP 41251 and UCN-01) are described in the literature [see for example, Gescher A., Gen Pharmacol. 1998, 31, p721-8].

Synthesis of 5'-deoxy-5-thio-adenosine (4)

5'-Deoxy-5-thio-adenosine (4) is a known compound [45] and it can be prepared readily from commercially available 2',3'-isopropylideneadenosine 1 as shown in *Scheme 1* [46].



1 2 3 4

Scheme 1

5'-Deoxy-5'-acetylthio-2',3'-O-isopropylideneadenosine (2)

Diethyl azodicarboxyl-ate (3.4 mL, 21.73 mmol) was added drop-wise over 5 min to an ice-cold solution of triphenylphosphine (5.7 g, 21.73 mmol). The solution was stirred for 30 min at 0 °C prior to the addition of 2',3'-*O*-isopropylideneadenosine (1; 3.0 g, 9.76 mmol) and stirring was then continued for a further 10 min to produce a yellow suspension. To the suspension a solution of thioacetic acid (1.6 mL, 21.73 mmol) in absol tetrahydrofuran (5 mL) was added drop-wise and stirring was then continued for a further 1 h at 0 °C. During this time the yellow suspension became a darker yellow

solution. After stirring for 1 h the solvent was removed under reduced pressure and the resulting yellowish residue was purified by flash chromatography on silica gel [350 g, $CHCl_3$/THF (4:1 v/v) and then $CHCl_3/CH_3OH$ (9:1 v/v)]. The fractions containing the product were combined and the solvent removed under reduced pressure. The residue was dried *in vacuo* (0.5 mbar) to furnish pure protected thionucleoside **2** (3.2 g, 90 %) as a white foam; TLC R_f (CH_2Cl_2/CH_3OH, 9:1 v/v) = 0.6, mp = 56-57 °C; ^{1}H-NMR ($CDCl_3$): δ 1.39 (s, 6H, CH_3), 2.34 (s, 3H, $COCH_3$), 3.18 and 3.29 (AB part of ABX spectrum, $J_{5'a\text{-}H,4'\text{-}H} = J_{5'b\text{-}H,4'\text{-}H} = 6.5$ Hz, $J_{gem} = 13.5$ Hz, 2H, 5'a-H, 5'b-H), 4.34 (dt, $J_{4'\text{-}H,3'\text{-}H} = 3$ Hz, $J_{4'a\text{-}H,5a'\text{-}H} = J_{4'\text{-}H,5'b\text{-}H} = 7$ Hz, 1H, 4'-H), 4.97 (dd, $J_{3'\text{-}H,4'\text{-}H} = 3$ Hz, $J_{3'\text{-}H,2'\text{-}H} = 6.5$ Hz, 1H, 3'-H), 5.51 (dd, $J_{2'\text{-}H,1'\text{-}H} = 2$ Hz, $J_{2'\text{-}H,3'\text{-}H} = 6.5$ Hz, 1H, 2'-H), 6.07 (d, $J_{1'\text{-}H,2'\text{-}H} =$ Hz, 1H, 1'-H), 5.9 (s, br., 2H, NH_2), 7.90 (s, 1H, 8-H) and 8.36 (s, 1H, 2-H); ^{13}C-NMR ($CDCl_3$): δ 25.56 (q, CH_3), 27.33 (q, CH_3), 30.79 (q, $COCH_3$), 31.60 (t, C-5'), 84.24 (d, C-3'), 84.43 (d, C-2'), 86.47 (d, C-4'), 91.07 (d, C-1'), 114.75 (s, $C(CH_3)_2$), 120.53 (s, C-5), 140.09 (d, C-8), 149.42 (s, C-4), 153.45 (d, C-2), 155.92 (s, C-6) and 194.79 (s, CO); ESMS; *m/z*: 366.0 [M + H$^+$]; $[\alpha]_D$ ($CDCl_3$) = -13.2.

5'-Deoxy-5'acetyl-thioadenosine (3)

A solution of compound **2** (200 mg, 0.54 mmol) was stirred in a mixture of formic acid and water (10 ml, 1:1) at room temperature. The progress of the reaction was monitored by reversed-phase HPLC. After 50 h reaction time the solvent was evaporated under reduced pressure. Traces of formic acid were removed by co-evaporating 5 times with absolute ethanol to produce an off-white powder, which was purified by silica gel flash chromatography [30 g, CH_2Cl_2/CH_3OH (4:1 v/v)]. The fractions containing the product were combined, the solvent removed under reduced pressure and the product further dried *in vacuo* (0.5 mbar) to title compound **3** (150 mg, 86 %); TLC R_f (CH_2Cl_2:CH_3OH, 9:1 v/v) = 0.24; ^{1}H-NMR ($CDCl_3$): δ 2.32 (s, 3H, $COCH_3$), 3.15 and 3.34 (AB part of ABX spectrum, $J_{5'\text{-}H,4'\text{-}H} = 5.5$ Hz, $J_{5'b\text{-}H,}$ 4'-H = 7 Hz, $J_{gem} = 14$ Hz, 2H, 5'a-H, 5'b-H), 3.9 (ddd, $J_{4'\text{-}H,3'\text{-}H} = 3.5$ Hz, $J_{5'a\text{-}H,4'\text{-}H} = 6$ Hz, $J_{5'b\text{-}H,4'\text{-}H} = 7.5$ Hz, 1H, 4'-H), 4.08 (m, 1H, 3'-H), 4.76 (t, $J_{2'\text{-}H,1'\text{-}H} = J_{2'\text{-}H,3'\text{-}H} = J_{2'\text{-}H,2'\text{-}OH} = 6$ Hz, 1H, 2'-H), 5.37 (s, 1H, D_20 exchangeable, 3'-OH), 5.51 (s, 1H, D_20 exchangeable, 2'-OH), 5.85 (d, $J_{1'\text{-}H,2'\text{-}H} =$ 6 Hz, 1H, 1'-H), 7.28 (s, br., 2H, D_20 exchangeable, 6-NH_2), 8.14 (s, 1H, 2-H) and 8.53 (s, 1H, 8-H); ESMS; *m/z*: 326.5 [M + H$^+$].

5'-Deoxy-5'-thioadenosine (4)

To eliminate traces of oxygen, a mixture of CH_3OH/H_2O (5:2) was degassed by first passing nitrogen gas (for 15 min) and secondly ammonia gas (for 15 min) through the mixture. Nucleoside **3** (50 mg, 0.16 mmol) was solubilised in the ammonia-saturated CH_3OH/H_20 mixture (7 mL) under N_2, and the mixture stirred at 0 °C. After 1.5 h the reaction mixture was frozen using liquid nitrogen and the solvent removed by drying *in vacuo* to afford title compound **4** (25 mg, 55 %); TLC R_f (CH_2Cl_2/CH_3OH, 7:1 v/v) = 0.85; mp = 109-110 °C, ^{1}H-NMR [(D_6 DMSO)]: δ 2.57 (s, br., 1H, 5'-SH), 2.75-2.80 (m, 2H, 5'a-H, 5'b-H), 3.98 (dt, $J_{4'\text{-H, }3'\text{-H}} = 3$ Hz, $J_{4'\text{-H, }5'\text{a-H}} = J_{4'\text{-H, }5'\text{b-H}} = 6$ Hz, 1H, 4'-H), 4.18 (q, $J_{3'\text{-H, }2'\text{-H}} = J_{3'\text{-H, }4'\text{-H}} = J_{3'\text{-H, }3'\text{-OH}} = 4$ Hz, 1H, 3'-H), 4.78 (q, $J_{2'\text{-H, }1'\text{-H}} = J_{2'\text{-H, }3'\text{-H}} = J_{2'\text{-H, }2'\text{-OH}} = 5$ Hz, 1H, 2'-H), 5.28 (d, $J_{3'\text{-OH, }3'\text{-OH}} = 5$ Hz, 1H, 3'-OH), 5.48 (d, $J_{2'\text{-OH, }2'\text{-H}} = 6$ Hz, 1H, 2'-OH), 5.88 (d, $J_{1'\text{-H, }2'\text{-H}} = 6$ Hz, 1H, 1'-H), 7.28 (s, br., 2H, 6-NH_2), 8.14 (s, 1H, 2-H) and 8.35 (s, 1H, 8-H); ESMS; *m/z*: 283.92 [M + H^+]; $[\alpha]_D$ (DMSO) = -29.3.

Example 8

Inhibition of PLK1 enzymatic activity by adenosine, thioadenosines, and thiol-reactive compounds

Adenosine, N-ethylmaleimide, iodoacetamide, and thimerosal were obtained from Sigma Chemical Co. 2'-Thioadenosine was obtained from Calbiochem. 5'-Thioadenosine was prepared as described in*Example 7*. All compounds were made up as 10 mM stocks in neat dimethylsulfoxide and fresh dilutions to the desired concentrations were made in assay buffer prior to the assay. The candidate compounds were incubated with the enzyme in the kinase assay buffer for the duration of the assay, usually 1 hour at 30 °C (refer *Example 4)*. For each compound duplicate samples, one of which contained dithiothreitol (DTT) at 1 mM final concentration, were assayed. The results are summarized in *Table 3* and *Figure 5*.

Example 9

Inhibition of PLK1 enzymatic activity by other small molecules

The effects of staurosporine, a promiscuous kinase inhibitor, and wortmannin, a specific PI-3 kinase inhibitor, were also tested for the inhibition of PLK1 activity. The

results showed that while staurosporine caused moderate inhibition of PLK1, wortmannin was considerably more potent, with a very similar activity to that reported for its PI-3 kinase inhibition. The PLK1 IC_{50} values for staurosporine and wortmannin in the biochemical assay were 0.8 ± 0.2 and 0.18 ± 0.1 μM, respectively (*Figure 8*).

In order further to investigate the possibility of other protein kinase inhibitors affecting PLK1 enzymatic activity, a library of trisubstituted purine CDK2 inhibitors was tested in the *in vitro* assay. It was found that purvalanol A, a potent ATP antagonist of several CDKs also inhibited PLK1 with an activity (IC_{50}) of 5 μM.

Example 10

Kinetic analysis of PLK1 inhibition by staurosporine and wortmannin

In order to determine the nature of inhibition of PLK1 activity by staurosporine and wortmannin, a full investigation of the dependence on ATP concentration of the inhibition by these two compounds was carried out (*Figure 9*). The results obtained showed that staurosporine inhibition was a fully ATP-competitive, whereas that of wortmannin was completely ATP-independent. This situation mirrors the previously reported mechanism of inhibition of PI-3 kinase by wortmannin through irreversible covalent modification of Lys833 in the ATP-binding site [37]. Staurosporine, on the other hand, was also reported to be less potent against PI-3 kinase (IC_{50} of 10 μM) [37].

Example 11

Flavonoids inhibit PLK1 activity *in vitro*

Based on the results clearly demonstrating that wortmannin is very potent against PLK1, we sought to test whether any other known PI3 kinase inhibitors have an effect on PLK1 activity. A number of flavonoid compounds including LY294002, Quercetin and Myricetin which were previously reported to cause a moderate inhibition of PI3 kinase activity (IC_{50} values of 1.4, 3.8 and 1.8μM respectively, [37]) were screened against PLK1 (*Table 12*). Interestingly, the results showed that indeed LY294002 was equally potent against PLK1 giving an IC50 value of 5-10 μM. Quercetin on the other hand was less potent (64 μM) whilst Myricetin was inactive against PLK1 (>100 μM IC_{50}).

Table 13 shows a summary of screening of 8 additional flavonoid compounds against PLK1. Of these morin hydrate was the most potent with an IC_{50} of 12 μM.

As dose-response inhibition for a number of closely related flavonoid inhibitors was obtained, it was possible to determine a structure-activity relationship for this compound class. Each of the other 10 compounds screened contains an identical core structure to morin and only vary on the extent of hydroxyl substitutions on the flavonoid. Comparing the inactive inhibitor, datescetin with morin, reveals that the R3' hydroxyl is important for binding (since it is absent in Datescetin). The lower potency of quercetin on PLK1 (64 μM) and its lack of a R1' hydroxyl also suggests that it makes intermolecular contacts in the ATP cleft. The lack of inhibition of myricetin and kaepmpferol which also lack this group is consistent this observation although it is likely that the additional OH group at R2' in myricetin interferes with binding. Comparison of luteolin with the weak inhibitor, quercetin suggests that the R3 hydroxyl makes a contribution due to the absence of this group in the former compounds. The inactivity of gangolin, which has no substituents on the 2nd ring is expected, however the weak inhibition of robinetin is unusual. This compound is similar to the inactive myricetin however does not have an R1 hydroxyl suggesting that this group makes unfavourable interactions and removing it results in tighter interaction. The weak inhibition observed for robinetin is probably at the threshold of sensitivity of the kinase assay and therefore may not be reliable. The inactivity of daidzein, fisetin and kaempferide is in line with the impotency of other similar compounds in this series.

In addition, based on literature reports [36] we found that out of 25 kinases tested, Casein Kinase II was the second most sensitive to inhibition by LY294002. The effects of wortmannin and LY294002 against Casein kinase II were tested and compared that to PLK1 inhibition (*Figure 10*).

Example 12

Sequence and structural comparison of PLK1 with other protein kinases

In order to obtain more information on the kinase domain of PLK1 and further characterise the residues that comprise the ATP binding pocket, a sequence similarity and homology analysis was performed (*Figure 3*). A FASTA search of protein kinases with available 3-D structural information revealed that the closest structural matches for the kinase domain included Cdk2 and ERK2, however the AGC kinase, PKA had the highest homology (over 40% similarity and 30% identity) As a consequence of the similarities of PLK1 and PKA, several commonly used PKA inhibitors were tested to determine if any correlation exists between the structural similarities and mode of inhibition of these two enzymes.

To this end, commercially available PKA inhibitors H89, A3 hydrochloride, KT5720 and 4-cyano 3-methylisoquinoline were screened against PLK1 and the results were compared to the published values against PKA. Surprisingly, none of these compounds caused any inhibition of PLK1, even at concentrations as high as 1mM. Moreover, Balanol a very potent inhibitor of the ACG family of protein kinases [47] was tested here to show no detectable inhibition of PLK1. Put together, these result clearly demonstrate that despite the fact the PLK1 has the greatest homology with PKA, their mode and mechanism of inhibition by small molecule ATP competitors appear to be vastly different (*Table 14*).

Example 13

Molecular Modelling of the interactions of inhibitors with PLK1 kinase domain

As mentioned above, the closest structural homologue to the kinase domain of PLK1 is protein kinase A. Despite the relatively low sequence identity between these two enzymes, the structural conservation of the protein kinase fold allowed the construction of a homology model structure of PLK1. This hypothetical structure was then used in flexible docking calculations with the identified PLK1 ATP competitive ligands to determine if representative kinase binding modes could be identified and thus enable validation of model. Positioning of the trisubstituted purine derivative, purvalanol A was undertaken using the automated docking routine, Affinity (I2000, Accelrys) that

allows for flexibility in both the receptor binding site and in the ligand itself. The use of this ligand is expedient as it is a potent Cdk2 inhibitor and its complex crystal structure has been previously determined. While it is possible that purvalanol A binds to PLK1 in a different way, its Cdk2 pose is nonetheless suggestive of how the purines interact with the mitotic kinase. Investigation of numerous predicted structures of purvalanol A with PLK1 indeed revealed an energetically favourable pose that formed similar contacts to those observed in the Cdk2 bound structure (*Figure 11A*).

The hinge region H-bonds observed in the Cdk2 complex (E81, L83) were formed with C133 of PLK1 and in addition the isopropyl group interacts with the deep cleft of the ATP pocket (L130 corresponding to F80 in Cdk2). As a cross-validation, purvalanol A was also docked into the structure of PKA that was used as the template for the PLK1 model. This result confirmed that no binding mode forming kinase inhibitory contacts was observed with PKA and therefore was consistent with the lack of inhibition of this inhibitor. In order to probe the structural basis for the lower potency of staurosporine against PLK1, this compounds was modelled into the homology structure. A similar binding mode to that observed in Cdk2 was observed. Wortmannin also was modelled in the ATP cleft of the PLK1 homology structure to determine if the structural basis for its irreversible inhibition could be predicted. Docking of this inhibitor revealed an energetically favourable binding mode that placed the reactive functionality in close proximity to K82 of PLK1. Formation of the covalent bond between Wortmannin and K82, followed by energy minimisation to convergence resulted in a plausible low energy complex structure that was consistent with its interactions in the PI3 kinase experimental structure (*Figure 12*).

In order to further examine, the interactions of the newly characterised PLK1 inhibitors, the flavonoid compound LY294002 was additionally docked into the PLK1 kinase domain. As this compound has been developed as a PI3 kinase inhibitor and since its co-crystal structure has been solved, a useful benchmark is available to probe the model structure. This time however, comparison of the structural ensemble of docked poses showed that no energetically realistic binding mode closely representing that observed with PI3K. Comparison of the primary structure of PI3K and PLK1 shows that these

two enzymes have a low sequence identity (15%) and diverge considerably in the residues lining the ATP cleft. It is thus very possible that LY294002 forms different non-bonded interactions in the PLK1 context. Evaluation of the most energetically favourable structure for this inhibitor indicates a plausible binding mode with the PLK1 catalytic domain however is substantially different from the binding mode observed in the PI3K structure.

Due to the observed activity of morin hydrate on PLK1 and since activity data was available for a number of close structural analogues, this compound was additionally docked into the PLK1 kinase domain. Examination of the structural ensemble generated by molecular dynamics docking indicates that energetically plausible poses representative of "kinase inhibitors" from crystal structures are observed and are consistent with the activities of other molecules in this series (*Figure 11B*).

Example 14

ATP-dependence of PLK1 inhibition by 5'-thioadenosine

The kinase assay described in *Example 4* was used. ATP dependence of the effects of adenosine, 2'-thioadenosine, 5-'thioadenosine, and thimerosal was investigated at 12.5, 25, 50, and 100 μM ATP. The results showed that none of these compounds were classical competitive inhibitors with respect to ATP, as would be expected from a covalent inhibitor. Results of the kinetic analysis with 5'-thioadenosine are shown in *Figure 6*.

Example 15

Contact models of PLK1 kinase domain with bound ligands

The homology model described in *Example 1* was used as the basis for the docking of ATP, 5'-thioadenosine, and two additional ATP-competitive kinase inhibitors we have found to inhibit PLK1. The conformations of these ligands in the PLK1 ATP-binding pocket are depicted in *Figure 7*. Descriptions of the PLK1-ligand complex structures in the form of interatomic distances between the residues lining the ATP-binding pocket of PLK1 and the ligands were obtained using the molecular modelling programs Quanta2000 (Accelrys, CA, USA) and Maestro (Schrodinger Inc., Oregon, USA). The

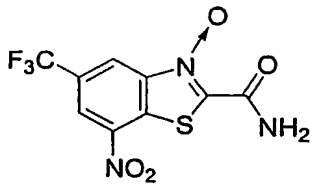
output from the former lists all contacts between PLK1 and ligands that are less than 3.5 Å. In the latter case a listing of all PLK1-ligand contacts not involving H atoms is given, together with the interatomic distances. Also given is a measure of the quality of the contacts. Only favourable contacts are listed and the closer the value of the contact cut-off ratio to 1.3, the better the contact. Results are summarized in *Table 4* (Maestro) & *Table 5* (Quanta) for ATP, in *Table 6* (Maestro) & *Table 7* (Quanta) for 5'-thioadenosine, in *Table 8* (Maestro) & *Table 9* (Quanta) for staurosporine, and in *Table 10* (Maestro) & *Table 11* (Quanta) for 4-[4-(4-methyl-2-methylamino-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol. The ligand atom numbering is shown in *Figure 7.*

Example 16

Covalent inhibition of PLK1 by benzthiazole N-oxide derivative

The homology model of the invention was further validated by studies using two known inhibitors of PLK, Inhibitors A and B, the structures of which are shown below.

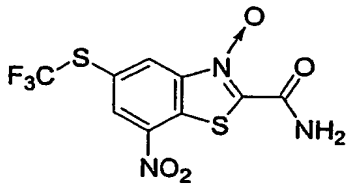
As is shown in *Figure 13*, the selective PLK1 inhibitor A (IC_{50} for PLK1 activity is 0.5 μM at 10 μM ATP) competes with ATP for binding to the active site of the enzyme. Furthermore, upon varying the concentration of inhibitor as well as of ATP, the kinetic analysis shows that the binding of the inhibitor is fully reversible, as the $K_{M,\ ATP}$ (intercepts on the abscissa in the Lineweaver-Burk plot) vary, with no change in the reaction velocity V_{max} of the enzyme (common intersect on the ordinate).



Inhibitor A: 7-Nitro-3-oxy-5-trifluoromethyl-benzothiazole-2-carboxylic acid amide

The closely related analogue Inhibitor B, which only differs from A by the presence of a SCF_3 group rather than a CF_3 group, shows different behaviour. The kinetic analysis for this compound suggests that the inhibitor affects the V_{max} of the enzyme, without

altering the apparent affinity for ATP ($K_{M, ATP}$) (*Figure 14*). This shows that the inhibitor is non-competitive with respect to ATP and hence strongly suggests that it is binding covalently to the PLK1 ATP binding site.



Inhibitor B: 7-Nitro-3-oxy-5-trifluoromethylsulfanyl-benzothiazole-2-carboxylic acid amide

This covalent binding would most likely be with the cysteine residue (C67) in the binding pocket of PLK1 and is supported through the close proximity of the potential reactive atoms of Inhibitor B to the cysteine in the modelled structure of inhibitor A shown in *Figure 15*.

Various modifications and variations of the invention will be apparent to those skilled in the art without departing from the scope and spirit of the invention. Although the invention has been described in connection with specific preferred embodiments, it should be understood that the invention as claimed should not be unduly limited to such specific embodiments. Indeed, various modifications of the described modes for carrying out the invention which are obvious to those skilled in the relevant fields are intended to be covered by the present invention.

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Table 1. Sequence comparison between PLK1 and CDK2, ERK-2, or PKA kinase domains, respectively.

PLK1 sequence segment	Sequence identity (%)		
	CDK2	*ERK-2*	*PKA*
1–50	0	8	12
51–100	14	20	28
101–150	18	8	20
151–200	44	48	44
201–250	30	30	42
251–306	18	20	22

Table 2. PDB coordinate file of PLK1-ATP homology model

ATOM	1	N	ARG	52	108.414	117.322	91.897	1.00	0.00	N
ATOM	2	CA	ARG	52	109.182	116.827	90.698	1.00	0.00	C
ATOM	3	C	ARG	52	108.390	116.045	89.578	1.00	0.00	C
ATOM	4	O	ARG	52	108.985	115.798	88.530	1.00	0.00	O
ATOM	5	CB	ARG	52	110.589	116.233	91.053	1.00	0.00	C
ATOM	6	CG	ARG	52	110.801	114.702	91.020	1.00	0.00	C
ATOM	7	CD	ARG	52	112.287	114.328	91.157	1.00	0.00	C
ATOM	8	NE	ARG	52	112.450	112.916	90.739	1.00	0.00	N
ATOM	9	CZ	ARG	52	113.551	112.190	90.870	1.00	0.00	C
ATOM	10	NH1	ARG	52	114.666	112.630	91.370	1.00	0.00	N
ATOM	11	NH2	ARG	52	113.501	110.971	90.474	1.00	0.00	N
ATOM	12	1H	ARG	52	107.626	116.687	92.087	1.00	0.00	H
ATOM	13	2H	ARG	52	109.037	117.350	92.717	1.00	0.00	H
ATOM	14	HE	ARG	52	111.635	112.458	90.308	1.00	0.00	H
ATOM	15	HA	ARG	52	109.432	117.749	90.134	1.00	0.00	H
ATOM	16	1HB	ARG	52	111.303	116.678	90.331	1.00	0.00	H
ATOM	17	2HB	ARG	52	110.945	116.616	92.029	1.00	0.00	H
ATOM	18	1HG	ARG	52	110.209	114.203	91.813	1.00	0.00	H
ATOM	19	2HG	ARG	52	110.408	114.292	90.070	1.00	0.00	H
ATOM	20	1HD	ARG	52	112.925	114.977	90.524	1.00	0.00	H
ATOM	21	2HD	ARG	52	112.620	114.481	92.204	1.00	0.00	H
ATOM	22	2HH1	ARG	52	114.619	113.601	91.675	1.00	0.00	H
ATOM	23	1HH1	ARG	52	115.438	111.966	91.428	1.00	0.00	H
ATOM	24	1HH2	ARG	52	112.572	110.717	90.120	1.00	0.00	H
ATOM	25	2HH2	ARG	52	114.330	110.391	90.596	1.00	0.00	H
ATOM	26	N	TYR	53	107.105	115.659	89.725	1.00	0.00	N
ATOM	27	CA	TYR	53	106.360	114.857	88.698	1.00	0.00	C
ATOM	28	C	TYR	53	104.944	115.448	88.356	1.00	0.00	C
ATOM	29	O	TYR	53	104.213	115.917	89.234	1.00	0.00	O
ATOM	30	CB	TYR	53	106.221	113.387	89.193	1.00	0.00	C
ATOM	31	CG	TYR	53	107.481	112.506	89.105	1.00	0.00	C
ATOM	32	CD1	TYR	53	108.238	112.270	90.254	1.00	0.00	C
ATOM	33	CD2	TYR	53	107.859	111.902	87.899	1.00	0.00	C
ATOM	34	CE1	TYR	53	109.362	111.450	90.197	1.00	0.00	C
ATOM	35	CE2	TYR	53	108.977	111.069	87.849	1.00	0.00	C
ATOM	36	CZ	TYR	53	109.729	110.848	89.000	1.00	0.00	C
ATOM	37	OH	TYR	53	110.838	110.047	88.972	1.00	0.00	O
ATOM	38	H	TYR	53	106.610	115.929	90.587	1.00	0.00	H
ATOM	39	HA	TYR	53	106.932	114.835	87.749	1.00	0.00	H
ATOM	40	1HB	TYR	53	105.807	113.374	90.220	1.00	0.00	H
ATOM	41	2HB	TYR	53	105.431	112.881	88.609	1.00	0.00	H
ATOM	42	HD1	TYR	53	107.971	112.729	91.194	1.00	0.00	H
ATOM	43	HD2	TYR	53	107.294	112.078	86.995	1.00	0.00	H
ATOM	44	HE1	TYR	53	109.966	111.296	91.080	1.00	0.00	H
ATOM	45	HE2	TYR	53	109.268	110.610	86.916	1.00	0.00	H
ATOM	46	HH	TYR	53	111.034	109.782	88.067	1.00	0.00	H
ATOM	47	N	VAL	54	104.539	115.358	87.076	1.00	0.00	N
ATOM	48	CA	VAL	54	103.182	115.765	86.588	1.00	0.00	C
ATOM	49	C	VAL	54	102.488	114.515	85.933	1.00	0.00	C
ATOM	50	O	VAL	54	102.989	113.950	84.954	1.00	0.00	O

ATOM	51	CB	VAL	54	103.294	116.991	85.608	1.00	0.00	C
ATOM	52	CG1	VAL	54	101.959	117.391	84.930	1.00	0.00	C
ATOM	53	CG2	VAL	54	103.822	118.277	86.288	1.00	0.00	C
ATOM	54	H	VAL	54	105.247	114.977	86.430	1.00	0.00	H
ATOM	55	HA	VAL	54	102.552	116.097	87.438	1.00	0.00	H
ATOM	56	HB	VAL	54	104.004	116.714	84.802	1.00	0.00	H
ATOM	57	1HG1	VAL	54	101.183	117.679	85.665	1.00	0.00	H
ATOM	58	2HG1	VAL	54	102.083	118.243	84.234	1.00	0.00	H
ATOM	59	3HG1	VAL	54	101.536	116.567	84.325	1.00	0.00	H
ATOM	60	2HG2	VAL	54	104.802	118.112	86.769	1.00	0.00	H
ATOM	61	3HG2	VAL	54	103.964	119.104	85.567	1.00	0.00	H
ATOM	62	1HG2	VAL	54	103.140	118.642	87.079	1.00	0.00	H
ATOM	63	N	ARG	55	101.311	114.102	86.439	0.00	0.00	N
ATOM	64	CA	ARG	55	100.503	113.002	85.830	0.00	0.00	C
ATOM	65	C	ARG	55	99.683	113.480	84.579	0.00	0.00	C
ATOM	66	O	ARG	55	98.913	114.441	84.665	0.00	0.00	O
ATOM	67	CB	ARG	55	99.533	112.395	86.882	0.00	0.00	C
ATOM	68	CG	ARG	55	100.151	111.773	88.159	0.00	0.00	C
ATOM	69	CD	ARG	55	99.092	111.038	88.997	0.00	0.00	C
ATOM	70	NE	ARG	55	99.641	110.761	90.348	0.00	0.00	N
ATOM	71	CZ	ARG	55	98.978	110.180	91.339	0.00	0.00	C
ATOM	72	NH1	ARG	55	97.772	109.704	91.239	0.00	0.00	N
ATOM	73	NH2	ARG	55	99.572	110.091	92.474	0.00	0.00	N
ATOM	74	HE	ARG	55	100.615	111.041	90.530	1.00	0.00	H
ATOM	75	H	ARG	55	100.954	114.668	87.214	0.00	0.00	H
ATOM	76	HA	ARG	55	101.187	112.185	85.519	0.00	0.00	H
ATOM	77	1HB	ARG	55	98.926	111.617	86.379	0.00	0.00	H
ATOM	78	2HB	ARG	55	98.793	113.166	87.182	0.00	0.00	H
ATOM	79	1HG	ARG	55	100.628	112.570	88.763	0.00	0.00	H
ATOM	80	2HG	ARG	55	100.970	111.072	87.909	0.00	0.00	H
ATOM	81	1HD	ARG	55	98.785	110.098	88.493	0.00	0.00	H
ATOM	82	2HD	ARG	55	98.176	111.658	89.090	0.00	0.00	H
ATOM	83	1HH1	ARG	55	97.371	109.276	92.070	0.00	0.00	H
ATOM	84	2HH1	ARG	55	97.378	109.802	90.301	0.00	0.00	H
ATOM	85	1HH2	ARG	55	99.060	109.677	93.250	0.00	0.00	H
ATOM	86	2HH2	ARG	55	100.498	110.524	92.448	0.00	0.00	H
ATOM	87	N	GLY	56	99.823	112.791	83.436	1.00	0.00	N
ATOM	88	CA	GLY	56	99.062	113.119	82.194	1.00	0.00	C
ATOM	89	C	GLY	56	97.780	112.295	81.942	1.00	0.00	C
ATOM	90	O	GLY	56	96.678	112.843	81.956	1.00	0.00	O
ATOM	91	H	GLY	56	100.528	112.039	83.459	1.00	0.00	H
ATOM	92	1HA	GLY	56	98.786	114.192	82.166	1.00	0.00	H
ATOM	93	2HA	GLY	56	99.729	112.995	81.322	1.00	0.00	H
ATOM	94	N	ARG	57	97.923	110.991	81.655	1.00	0.00	N
ATOM	95	CA	ARG	57	96.765	110.087	81.374	1.00	0.00	C
ATOM	96	C	ARG	57	97.000	108.655	81.967	1.00	0.00	C
ATOM	97	O	ARG	57	98.134	108.174	82.064	1.00	0.00	O
ATOM	98	CB	ARG	57	96.526	110.079	79.834	1.00	0.00	C
ATOM	99	CG	ARG	57	95.213	109.398	79.373	1.00	0.00	C
ATOM	100	CD	ARG	57	94.996	109.479	77.856	1.00	0.00	C
ATOM	101	NE	ARG	57	93.701	108.821	77.548	1.00	0.00	N
ATOM	102	CZ	ARG	57	93.241	108.542	76.337	1.00	0.00	C
ATOM	103	NH1	ARG	57	93.863	108.827	75.232	1.00	0.00	N
ATOM	104	NH2	ARG	57	92.101	107.952	76.262	1.00	0.00	N
ATOM	105	HE	ARG	57	93.108	108.556	78.347	1.00	0.00	H
ATOM	106	H	ARG	57	98.881	110.643	81.765	1.00	0.00	H
ATOM	107	HA	ARG	57	95.857	110.497	81.863	1.00	0.00	H
ATOM	108	1HB	ARG	57	96.511	111.124	79.467	1.00	0.00	H
ATOM	109	2HB	ARG	57	97.390	109.607	79.326	1.00	0.00	H
ATOM	110	1HG	ARG	57	95.204	108.329	79.670	1.00	0.00	H
ATOM	111	2HG	ARG	57	94.345	109.854	79.890	1.00	0.00	H
ATOM	112	1HD	ARG	57	94.981	110.534	77.515	1.00	0.00	H
ATOM	113	2HD	ARG	57	95.830	108.976	77.325	1.00	0.00	H
ATOM	114	2HH1	ARG	57	94.757	109.292	75.385	1.00	0.00	H
ATOM	115	1HH1	ARG	57	93.404	108.559	74.363	1.00	0.00	H
ATOM	116	1HH2	ARG	57	91.716	107.762	77.189	1.00	0.00	H
ATOM	117	2HH2	ARG	57	91.741	107.720	75.338	1.00	0.00	H
ATOM	118	N	PHE	58	95.918	107.949	82.336	1.00	0.00	N
ATOM	119	CA	PHE	58	95.987	106.512	82.726	1.00	0.00	C
ATOM	120	C	PHE	58	96.279	105.555	81.519	1.00	0.00	C
ATOM	121	O	PHE	58	95.611	105.617	80.481	1.00	0.00	O
ATOM	122	CB	PHE	58	94.718	106.129	83.545	1.00	0.00	C
ATOM	123	CG	PHE	58	93.362	106.079	82.812	1.00	0.00	C

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ATOM    124  CD1 PHE    58      92.925 104.888  82.221  1.00  0.00           C
ATOM    125  CE1 PHE    58      91.712 104.847  81.539  1.00  0.00           C
ATOM    126  CZ  PHE    58      90.924 105.992  81.449  1.00  0.00           C
ATOM    127  CE2 PHE    58      91.347 107.179  82.043  1.00  0.00           C
ATOM    128  CD2 PHE    58      92.561 107.221  82.725  1.00  0.00           C
ATOM    129  H   PHE    58      95.026 108.372  82.064  1.00  0.00           H
ATOM    130  HA  PHE    58      96.818 106.419  83.454  1.00  0.00           H
ATOM    131 1HB  PHE    58      94.904 105.145  84.019  1.00  0.00           H
ATOM    132 2HB  PHE    58      94.636 106.807  84.415  1.00  0.00           H
ATOM    133  HD1 PHE    58      93.540 103.999  82.262  1.00  0.00           H
ATOM    134  HE1 PHE    58      91.388 103.929  81.068  1.00  0.00           H
ATOM    135  HZ  PHE    58      89.986 105.961  80.913  1.00  0.00           H
ATOM    136  HE2 PHE    58      90.738 108.067  81.966  1.00  0.00           H
ATOM    137  HD2 PHE    58      92.882 108.149  83.179  1.00  0.00           H
ATOM    138  N   LEU    59      97.255 104.662  81.698  0.00  0.00           N
ATOM    139  CA  LEU    59      97.536 103.546  80.752  0.00  0.00           C
ATOM    140  C   LEU    59      96.581 102.327  81.038  0.00  0.00           C
ATOM    141  O   LEU    59      95.715 102.031  80.211  0.00  0.00           O
ATOM    142  CB  LEU    59      99.079 103.309  80.853  0.00  0.00           C
ATOM    143  CG  LEU    59      99.808 102.416  79.817  0.00  0.00           C
ATOM    144  CD1 LEU    59      99.468 100.925  79.926  0.00  0.00           C
ATOM    145  CD2 LEU    59      99.633 102.897  78.369  0.00  0.00           C
ATOM    146  H   LEU    59      97.696 104.671  82.627  0.00  0.00           H
ATOM    147  HA  LEU    59      97.324 103.877  79.716  0.00  0.00           H
ATOM    148 1HB  LEU    59      99.334 102.939  81.865  0.00  0.00           H
ATOM    149 2HB  LEU    59      99.594 104.291  80.798  0.00  0.00           H
ATOM    150  HG  LEU    59     100.892 102.501  80.047  0.00  0.00           H
ATOM    151 1HD1 LEU    59      99.582 100.542  80.956  0.00  0.00           H
ATOM    152 2HD1 LEU    59      98.436 100.688  79.606  0.00  0.00           H
ATOM    153 3HD1 LEU    59     100.153 100.321  79.304  0.00  0.00           H
ATOM    154 1HD2 LEU    59     100.279 102.327  77.675  0.00  0.00           H
ATOM    155 2HD2 LEU    59      98.592 102.786  78.012  0.00  0.00           H
ATOM    156 3HD2 LEU    59      99.915 103.961  78.256  0.00  0.00           H
ATOM    157  N   GLY    60      96.676 101.691  82.223  0.00  0.00           N
ATOM    158  CA  GLY    60      95.847 100.505  82.595  0.00  0.00           C
ATOM    159  C   GLY    60      95.373 100.470  84.075  0.00  0.00           C
ATOM    160  O   GLY    60      95.769 101.287  84.920  0.00  0.00           O
ATOM    161  H   GLY    60      97.447 102.031  82.805  0.00  0.00           H
ATOM    162 1HA  GLY    60      96.432  99.582  82.395  0.00  0.00           H
ATOM    163 2HA  GLY    60      94.967 100.400  81.931  0.00  0.00           H
ATOM    164  N   LYS    61      94.466  99.529  84.393  1.00  0.00           N
ATOM    165  CA  LYS    61      93.868  99.405  85.758  1.00  0.00           C
ATOM    166  C   LYS    61      93.299  97.972  86.042  1.00  0.00           C
ATOM    167  O   LYS    61      92.266  97.584  85.486  1.00  0.00           O
ATOM    168  CB  LYS    61      92.744 100.472  85.958  1.00  0.00           C
ATOM    169  CG  LYS    61      92.217 100.597  87.406  1.00  0.00           C
ATOM    170  CD  LYS    61      91.152 101.703  87.529  1.00  0.00           C
ATOM    171  CE  LYS    61      90.610 101.830  88.958  1.00  0.00           C
ATOM    172  NZ  LYS    61      89.603 102.910  89.003  1.00  0.00           N
ATOM    173 1HZ  LYS    61      89.236 102.999  89.961  1.00  0.00           H
ATOM    174 2HZ  LYS    61      90.040 103.799  88.719  1.00  0.00           H
ATOM    175 3HZ  LYS    61      88.831 102.687  88.359  1.00  0.00           H
ATOM    176  H   LYS    61      94.523  98.723  83.745  1.00  0.00           H
ATOM    177  HA  LYS    61      94.668  99.606  86.500  1.00  0.00           H
ATOM    178 1HB  LYS    61      93.112 101.471  85.646  1.00  0.00           H
ATOM    179 2HB  LYS    61      91.900 100.252  85.275  1.00  0.00           H
ATOM    180 1HG  LYS    61      91.791  99.629  87.739  1.00  0.00           H
ATOM    181 2HG  LYS    61      93.058 100.804  88.098  1.00  0.00           H
ATOM    182 1HD  LYS    61      91.583 102.672  87.205  1.00  0.00           H
ATOM    183 2HD  LYS    61      90.322 101.497  86.825  1.00  0.00           H
ATOM    184 1HE  LYS    61      90.160 100.873  89.292  1.00  0.00           H
ATOM    185 2HE  LYS    61      91.431 102.052  89.669  1.00  0.00           H
ATOM    186  N   GLY    62      93.868  97.257  87.026  0.00  0.00           N
ATOM    187  CA  GLY    62      93.338  95.929  87.443  0.00  0.00           C
ATOM    188  C   GLY    62      93.782  95.448  88.844  0.00  0.00           C
ATOM    189  O   GLY    62      93.881  96.219  89.801  0.00  0.00           O
ATOM    190  H   GLY    62      94.799  97.595  87.296  0.00  0.00           H
ATOM    191 1HA  GLY    62      93.630  95.190  86.668  0.00  0.00           H
ATOM    192 2HA  GLY    62      92.228  95.918  87.437  0.00  0.00           H
ATOM    193  N   GLY    63      94.055  94.138  88.968  1.00  0.00           N
ATOM    194  CA  GLY    63      94.411  93.510  90.288  1.00  0.00           C
ATOM    195  C   GLY    63      95.817  93.707  90.924  1.00  0.00           C
ATOM    196  O   GLY    63      96.231  92.889  91.746  1.00  0.00           O
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ATOM	197	H	GLY	63	93.953	93.598	88.103	1.00	0.00	H
ATOM	198	1HA	GLY	63	93.677	93.819	91.056	1.00	0.00	H
ATOM	199	2HA	GLY	63	94.259	92.418	90.203	1.00	0.00	H
ATOM	200	N	PHE	64	96.503	94.806	90.594	0.00	0.00	N
ATOM	201	CA	PHE	64	97.650	95.340	91.383	0.00	0.00	C
ATOM	202	C	PHE	64	97.219	96.766	91.873	0.00	0.00	C
ATOM	203	O	PHE	64	96.780	96.906	93.017	0.00	0.00	O
ATOM	204	CB	PHE	64	98.957	95.211	90.531	0.00	0.00	C
ATOM	205	CG	PHE	64	100.322	95.180	91.262	0.00	0.00	C
ATOM	206	CD1	PHE	64	101.339	94.374	90.729	0.00	0.00	C
ATOM	207	CE1	PHE	64	102.589	94.313	91.339	0.00	0.00	C
ATOM	208	CZ	PHE	64	102.844	95.070	92.476	0.00	0.00	C
ATOM	209	CE2	PHE	64	101.849	95.880	93.015	0.00	0.00	C
ATOM	210	CD2	PHE	64	100.597	95.943	92.407	0.00	0.00	C
ATOM	211	H	PHE	64	96.013	95.366	89.888	0.00	0.00	H
ATOM	212	HA	PHE	64	97.815	94.744	92.306	0.00	0.00	H
ATOM	213	1HB	PHE	64	98.995	95.988	89.745	0.00	0.00	H
ATOM	214	2HB	PHE	64	98.885	94.272	89.943	0.00	0.00	H
ATOM	215	HD1	PHE	64	101.175	93.786	89.834	0.00	0.00	H
ATOM	216	HE1	PHE	64	103.371	93.687	90.923	0.00	0.00	H
ATOM	217	HZ	PHE	64	103.822	95.022	92.935	0.00	0.00	H
ATOM	218	HE2	PHE	64	102.058	96.458	93.903	0.00	0.00	H
ATOM	219	HD2	PHE	64	99.845	96.585	92.839	0.00	0.00	H
ATOM	220	N	ALA	65	97.243	97.795	90.990	1.00	0.00	N
ATOM	221	CA	ALA	65	96.401	99.013	91.144	1.00	0.00	C
ATOM	222	C	ALA	65	96.155	99.807	89.814	1.00	0.00	C
ATOM	223	O	ALA	65	95.088	99.660	89.208	1.00	0.00	O
ATOM	224	CB	ALA	65	96.915	99.890	92.311	1.00	0.00	C
ATOM	225	H	ALA	65	97.644	97.519	90.086	1.00	0.00	H
ATOM	226	HA	ALA	65	95.375	98.686	91.416	1.00	0.00	H
ATOM	227	2HB	ALA	65	96.805	99.369	93.278	1.00	0.00	H
ATOM	228	3HB	ALA	65	97.986	100.139	92.197	1.00	0.00	H
ATOM	229	1HB	ALA	65	96.357	100.841	92.391	1.00	0.00	H
ATOM	230	N	LYS	66	97.056	100.720	89.405	1.00	0.00	N
ATOM	231	CA	LYS	66	96.846	101.620	88.233	1.00	0.00	C
ATOM	232	C	LYS	66	98.200	102.188	87.702	1.00	0.00	C
ATOM	233	O	LYS	66	98.947	102.808	88.469	1.00	0.00	O
ATOM	234	CB	LYS	66	95.815	102.752	88.564	1.00	0.00	C
ATOM	235	CG	LYS	66	96.230	103.839	89.590	1.00	0.00	C
ATOM	236	CD	LYS	66	95.060	104.754	89.991	1.00	0.00	C
ATOM	237	CE	LYS	66	95.529	105.928	90.862	1.00	0.00	C
ATOM	238	NZ	LYS	66	94.373	106.785	91.189	1.00	0.00	N
ATOM	239	1HZ	LYS	66	94.684	107.574	91.773	1.00	0.00	H
ATOM	240	2HZ	LYS	66	93.956	107.146	90.319	1.00	0.00	H
ATOM	241	3HZ	LYS	66	93.670	106.234	91.702	1.00	0.00	H
ATOM	242	H	LYS	66	97.952	100.685	89.906	1.00	0.00	H
ATOM	243	HA	LYS	66	96.407	101.006	87.418	1.00	0.00	H
ATOM	244	1HB	LYS	66	95.539	103.250	87.615	1.00	0.00	H
ATOM	245	2HB	LYS	66	94.875	102.272	88.900	1.00	0.00	H
ATOM	246	1HG	LYS	66	96.657	103.368	90.497	1.00	0.00	H
ATOM	247	2HG	LYS	66	97.055	104.444	89.163	1.00	0.00	H
ATOM	248	1HD	LYS	66	94.549	105.136	89.086	1.00	0.00	H
ATOM	249	2HD	LYS	66	94.294	104.158	90.526	1.00	0.00	H
ATOM	250	1HE	LYS	66	96.013	105.558	91.789	1.00	0.00	H
ATOM	251	2HE	LYS	66	96.299	106.524	90.330	1.00	0.00	H
ATOM	252	N	CYS	67	98.478	102.033	86.400	1.00	0.00	N
ATOM	253	CA	CYS	67	99.654	102.670	85.746	1.00	0.00	C
ATOM	254	C	CYS	67	99.278	103.971	84.964	1.00	0.00	C
ATOM	255	O	CYS	67	98.198	104.091	84.372	1.00	0.00	O
ATOM	256	CB	CYS	67	100.379	101.592	84.922	1.00	0.00	C
ATOM	257	SG	CYS	67	99.311	100.811	83.669	1.00	0.00	S
ATOM	258	H	CYS	67	97.759	101.563	85.832	1.00	0.00	H
ATOM	259	HA	CYS	67	100.393	102.962	86.518	1.00	0.00	H
ATOM	260	1HB	CYS	67	101.271	102.013	84.418	1.00	0.00	H
ATOM	261	2HB	CYS	67	100.767	100.803	85.593	1.00	0.00	H
ATOM	262	HG	CYS	67	100.236	100.000	83.152	1.00	0.00	H
ATOM	263	N	PHE	68	100.157	104.979	85.038	1.00	0.00	N
ATOM	264	CA	PHE	68	99.953	106.316	84.412	1.00	0.00	C
ATOM	265	C	PHE	68	101.159	106.726	83.511	1.00	0.00	C
ATOM	266	O	PHE	68	102.314	106.458	83.840	1.00	0.00	O
ATOM	267	CB	PHE	68	99.753	107.364	85.554	1.00	0.00	C
ATOM	268	CG	PHE	68	98.298	107.699	85.907	1.00	0.00	C
ATOM	269	CD1	PHE	68	97.740	108.912	85.487	1.00	0.00	C

ATOM	270	CE1	PHE	68	96.435	109.246	85.843	1.00	0.00	C
ATOM	271	CZ	PHE	68	95.682	108.371	86.620	1.00	0.00	C
ATOM	272	CE2	PHE	68	96.228	107.159	87.035	1.00	0.00	C
ATOM	273	CD2	PHE	68	97.532	106.823	86.682	1.00	0.00	C
ATOM	274	H	PHE	68	101.038	104.758	85.528	1.00	0.00	H
ATOM	275	HA	PHE	68	99.054	106.312	83.764	1.00	0.00	H
ATOM	276	1HB	PHE	68	100.300	107.066	86.470	1.00	0.00	H
ATOM	277	2HB	PHE	68	100.257	108.312	85.283	1.00	0.00	H
ATOM	278	HD1	PHE	68	98.312	109.598	84.877	1.00	0.00	H
ATOM	279	HE1	PHE	68	96.009	110.183	85.512	1.00	0.00	H
ATOM	280	HZ	PHE	68	94.669	108.628	86.896	1.00	0.00	H
ATOM	281	HE2	PHE	68	95.640	106.480	87.633	1.00	0.00	H
ATOM	282	HD2	PHE	68	97.947	105.882	87.013	1.00	0.00	H
ATOM	283	N	GLU	69	100.875	107.502	82.456	1.00	0.00	N
ATOM	284	CA	GLU	69	101.904	108.317	81.744	1.00	0.00	C
ATOM	285	C	GLU	69	102.269	109.587	82.591	1.00	0.00	C
ATOM	286	O	GLU	69	101.475	110.527	82.695	1.00	0.00	O
ATOM	287	CB	GLU	69	101.313	108.631	80.346	1.00	0.00	C
ATOM	288	CG	GLU	69	102.257	109.425	79.404	1.00	0.00	C
ATOM	289	CD	GLU	69	101.724	109.581	77.983	1.00	0.00	C
ATOM	290	OE1	GLU	69	101.463	108.612	77.239	1.00	0.00	O
ATOM	291	OE2	GLU	69	101.433	110.872	77.674	1.00	0.00	O
ATOM	292	H	GLU	69	99.870	107.688	82.316	1.00	0.00	H
ATOM	293	HA	GLU	69	102.816	107.705	81.581	1.00	0.00	H
ATOM	294	1HB	GLU	69	101.047	107.679	79.841	1.00	0.00	H
ATOM	295	2HB	GLU	69	100.356	109.179	80.447	1.00	0.00	H
ATOM	296	1HG	GLU	69	102.471	110.425	79.828	1.00	0.00	H
ATOM	297	2HG	GLU	69	103.236	108.929	79.306	1.00	0.00	H
ATOM	298	N	ILE	70	103.448	109.579	83.229	1.00	0.00	N
ATOM	299	CA	ILE	70	103.873	110.642	84.193	1.00	0.00	C
ATOM	300	C	ILE	70	105.179	111.309	83.637	1.00	0.00	C
ATOM	301	O	ILE	70	106.208	110.650	83.454	1.00	0.00	O
ATOM	302	CB	ILE	70	104.059	110.093	85.662	1.00	0.00	C
ATOM	303	CG1	ILE	70	102.877	109.225	86.195	1.00	0.00	C
ATOM	304	CG2	ILE	70	104.317	111.255	86.658	1.00	0.00	C
ATOM	305	CD1	ILE	70	103.026	108.633	87.611	1.00	0.00	C
ATOM	306	H	ILE	70	103.997	108.715	83.099	1.00	0.00	H
ATOM	307	HA	ILE	70	103.089	111.422	84.256	1.00	0.00	H
ATOM	308	HB	ILE	70	104.960	109.444	85.657	1.00	0.00	H
ATOM	309	1HG1	ILE	70	101.931	109.795	86.130	1.00	0.00	H
ATOM	310	2HG1	ILE	70	102.737	108.371	85.507	1.00	0.00	H
ATOM	311	2HG2	ILE	70	105.106	111.947	86.313	1.00	0.00	H
ATOM	312	3HG2	ILE	70	103.412	111.865	86.831	1.00	0.00	H
ATOM	313	1HG2	ILE	70	104.649	110.880	87.643	1.00	0.00	H
ATOM	314	2HD1	ILE	70	104.015	108.167	87.762	1.00	0.00	H
ATOM	315	3HD1	ILE	70	102.906	109.405	88.395	1.00	0.00	H
ATOM	316	1HD1	ILE	70	102.263	107.858	87.810	1.00	0.00	H
ATOM	317	N	SER	71	105.152	112.631	83.413	1.00	0.00	N
ATOM	318	CA	SER	71	106.376	113.412	83.098	1.00	0.00	C
ATOM	319	C	SER	71	107.154	113.834	84.385	1.00	0.00	C
ATOM	320	O	SER	71	106.586	114.421	85.309	1.00	0.00	O
ATOM	321	CB	SER	71	105.960	114.645	82.265	1.00	0.00	C
ATOM	322	OG	SER	71	107.110	115.366	81.807	1.00	0.00	O
ATOM	323	H	SER	71	104.293	113.093	83.746	1.00	0.00	H
ATOM	324	HA	SER	71	107.043	112.810	82.450	1.00	0.00	H
ATOM	325	1HB	SER	71	105.366	114.332	81.383	1.00	0.00	H
ATOM	326	2HB	SER	71	105.297	115.316	82.847	1.00	0.00	H
ATOM	327	HG	SER	71	107.585	115.699	82.578	1.00	0.00	H
ATOM	328	N	ASP	72	108.478	113.631	84.406	1.00	0.00	N
ATOM	329	CA	ASP	72	109.394	114.350	85.338	1.00	0.00	C
ATOM	330	C	ASP	72	109.438	115.878	84.976	1.00	0.00	C
ATOM	331	O	ASP	72	109.784	116.245	83.851	1.00	0.00	O
ATOM	332	CB	ASP	72	110.803	113.684	85.270	1.00	0.00	C
ATOM	333	CG	ASP	72	111.439	113.276	86.597	1.00	0.00	C
ATOM	334	OD1	ASP	72	111.932	112.171	86.785	1.00	0.00	O
ATOM	335	OD2	ASP	72	111.409	114.257	87.539	1.00	0.00	O
ATOM	336	H	ASP	72	108.829	113.054	83.626	1.00	0.00	H
ATOM	337	HA	ASP	72	108.993	114.230	86.367	1.00	0.00	H
ATOM	338	1HB	ASP	72	110.779	112.765	84.660	1.00	0.00	H
ATOM	339	2HB	ASP	72	111.527	114.326	84.736	1.00	0.00	H
ATOM	340	N	ALA	73	109.010	116.750	85.893	1.00	0.00	N
ATOM	341	CA	ALA	73	108.809	118.199	85.618	1.00	0.00	C
ATOM	342	C	ALA	73	110.090	119.067	85.378	1.00	0.00	C

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ATOM    343  O   ALA    73     110.112 119.894  84.466  1.00  0.00           O
ATOM    344  CB  ALA    73     107.957 118.712  86.796  1.00  0.00           C
ATOM    345  H   ALA    73     108.846 116.340  86.825  1.00  0.00           H
ATOM    346  HA  ALA    73     108.197 118.298  84.699  1.00  0.00           H
ATOM    347 2HB  ALA    73     107.046 118.105  86.956  1.00  0.00           H
ATOM    348 3HB  ALA    73     108.520 118.720  87.749  1.00  0.00           H
ATOM    349 1HB  ALA    73     107.622 119.748  86.618  1.00  0.00           H
ATOM    350  N   ASP    74     111.144 118.878  86.187  1.00  0.00           N
ATOM    351  CA  ASP    74     112.426 119.637  86.060  1.00  0.00           C
ATOM    352  C   ASP    74     113.439 119.098  84.983  1.00  0.00           C
ATOM    353  O   ASP    74     114.168 119.901  84.399  1.00  0.00           O
ATOM    354  CB  ASP    74     113.039 119.767  87.483  1.00  0.00           C
ATOM    355  CG  ASP    74     112.259 120.707  88.409  1.00  0.00           C
ATOM    356  OD1 ASP    74     112.543 121.888  88.568  1.00  0.00           O
ATOM    357  OD2 ASP    74     111.176 120.106  88.975  1.00  0.00           O
ATOM    358  H   ASP    74     110.954 118.227  86.954  1.00  0.00           H
ATOM    359  HA  ASP    74     112.196 120.667  85.713  1.00  0.00           H
ATOM    360 1HB  ASP    74     113.155 118.780  87.967  1.00  0.00           H
ATOM    361 2HB  ASP    74     114.063 120.175  87.408  1.00  0.00           H
ATOM    362  N   THR    75     113.491 117.782  84.701  0.00  0.00           N
ATOM    363  CA  THR    75     114.274 117.208  83.552  0.00  0.00           C
ATOM    364  C   THR    75     113.505 117.002  82.190  0.00  0.00           C
ATOM    365  O   THR    75     114.162 116.797  81.167  0.00  0.00           O
ATOM    366  CB  THR    75     114.958 115.866  83.972  0.00  0.00           C
ATOM    367  OG1 THR    75     114.001 114.890  84.377  0.00  0.00           O
ATOM    368  CG2 THR    75     116.000 115.964  85.096  0.00  0.00           C
ATOM    369  H   THR    75     112.860 117.204  85.264  0.00  0.00           H
ATOM    370  HA  THR    75     115.099 117.901  83.291  0.00  0.00           H
ATOM    371  HB  THR    75     115.494 115.471  83.084  0.00  0.00           H
ATOM    372  HG1 THR    75     114.468 114.041  84.362  0.00  0.00           H
ATOM    373 1HG2 THR    75     116.485 114.990  85.288  0.00  0.00           H
ATOM    374 2HG2 THR    75     116.800 116.685  84.847  0.00  0.00           H
ATOM    375 3HG2 THR    75     115.544 116.296  86.048  0.00  0.00           H
ATOM    376  N   LYS    76     112.156 117.002  82.157  1.00  0.00           N
ATOM    377  CA  LYS    76     111.326 116.626  80.966  1.00  0.00           C
ATOM    378  C   LYS    76     111.521 115.147  80.454  1.00  0.00           C
ATOM    379  O   LYS    76     111.955 114.899  79.326  1.00  0.00           O
ATOM    380  CB  LYS    76     111.377 117.750  79.890  1.00  0.00           C
ATOM    381  CG  LYS    76     110.215 117.715  78.869  1.00  0.00           C
ATOM    382  CD  LYS    76     110.269 118.893  77.878  1.00  0.00           C
ATOM    383  CE  LYS    76     109.083 118.874  76.902  1.00  0.00           C
ATOM    384  NZ  LYS    76     109.178 120.032  75.991  1.00  0.00           N
ATOM    385 1HZ  LYS    76     108.383 120.020  75.336  1.00  0.00           H
ATOM    386 2HZ  LYS    76     109.156 120.904  76.540  1.00  0.00           H
ATOM    387 3HZ  LYS    76     110.059 119.982  75.461  1.00  0.00           H
ATOM    388  H   LYS    76     111.732 117.241  83.060  1.00  0.00           H
ATOM    389  HA  LYS    76     110.283 116.647  81.335  1.00  0.00           H
ATOM    390 1HB  LYS    76     111.373 118.738  80.390  1.00  0.00           H
ATOM    391 2HB  LYS    76     112.350 117.701  79.362  1.00  0.00           H
ATOM    392 1HG  LYS    76     110.236 116.758  78.310  1.00  0.00           H
ATOM    393 2HG  LYS    76     109.246 117.726  79.405  1.00  0.00           H
ATOM    394 1HD  LYS    76     110.276 119.850  78.439  1.00  0.00           H
ATOM    395 2HD  LYS    76     111.226 118.866  77.323  1.00  0.00           H
ATOM    396 1HE  LYS    76     109.072 117.929  76.323  1.00  0.00           H
ATOM    397 2HE  LYS    76     108.124 118.910  77.455  1.00  0.00           H
ATOM    398  N   GLU    77     111.182 114.160  81.304  1.00  0.00           N
ATOM    399  CA  GLU    77     111.388 112.710  81.010  1.00  0.00           C
ATOM    400  C   GLU    77     110.056 111.924  81.242  1.00  0.00           C
ATOM    401  O   GLU    77     109.498 111.953  82.341  1.00  0.00           O
ATOM    402  CB  GLU    77     112.526 112.150  81.907  1.00  0.00           C
ATOM    403  CG  GLU    77     113.952 112.687  81.620  1.00  0.00           C
ATOM    404  CD  GLU    77     115.006 112.124  82.569  1.00  0.00           C
ATOM    405  OE1 GLU    77     115.199 112.545  83.706  1.00  0.00           O
ATOM    406  OE2 GLU    77     115.704 111.096  82.017  1.00  0.00           O
ATOM    407  H   GLU    77     110.912 114.507  82.230  1.00  0.00           H
ATOM    408  HA  GLU    77     111.698 112.563  79.954  1.00  0.00           H
ATOM    409 1HB  GLU    77     112.276 112.325  82.971  1.00  0.00           H
ATOM    410 2HB  GLU    77     112.548 111.047  81.804  1.00  0.00           H
ATOM    411 1HG  GLU    77     114.243 112.476  80.574  1.00  0.00           H
ATOM    412 2HG  GLU    77     113.973 113.790  81.706  1.00  0.00           H
ATOM    413  N   VAL    78     109.538 111.228  80.218  1.00  0.00           N
ATOM    414  CA  VAL    78     108.198 110.559  80.279  1.00  0.00           C
ATOM    415  C   VAL    78     108.278 109.046  80.702  1.00  0.00           C
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ATOM	416	O	VAL	78	109.020	108.243	80.129	1.00	0.00	O
ATOM	417	CB	VAL	78	107.372	110.787	78.964	1.00	0.00	C
ATOM	418	CG1	VAL	78	106.959	112.261	78.749	1.00	0.00	C
ATOM	419	CG2	VAL	78	108.015	110.259	77.661	1.00	0.00	C
ATOM	420	H	VAL	78	110.071	111.278	79.345	1.00	0.00	H
ATOM	421	HA	VAL	78	107.598	111.065	81.062	1.00	0.00	H
ATOM	422	HB	VAL	78	106.424	110.234	79.103	1.00	0.00	H
ATOM	423	1HG1	VAL	78	107.833	112.918	78.578	1.00	0.00	H
ATOM	424	2HG1	VAL	78	106.287	112.382	77.879	1.00	0.00	H
ATOM	425	3HG1	VAL	78	106.421	112.669	79.625	1.00	0.00	H
ATOM	426	2HG2	VAL	78	108.267	109.184	77.736	1.00	0.00	H
ATOM	427	3HG2	VAL	78	107.338	110.363	76.794	1.00	0.00	H
ATOM	428	1HG2	VAL	78	108.950	110.791	77.408	1.00	0.00	H
ATOM	429	N	PHE	79	107.458	108.656	81.701	1.00	0.00	N
ATOM	430	CA	PHE	79	107.559	107.335	82.387	1.00	0.00	C
ATOM	431	C	PHE	79	106.160	106.654	82.583	1.00	0.00	C
ATOM	432	O	PHE	79	105.163	107.290	82.943	1.00	0.00	O
ATOM	433	CB	PHE	79	108.193	107.551	83.793	1.00	0.00	C
ATOM	434	CG	PHE	79	109.667	107.986	83.837	1.00	0.00	C
ATOM	435	CD1	PHE	79	110.007	109.280	84.244	1.00	0.00	C
ATOM	436	CE1	PHE	79	111.344	109.666	84.309	1.00	0.00	C
ATOM	437	CZ	PHE	79	112.347	108.773	83.948	1.00	0.00	C
ATOM	438	CE2	PHE	79	112.018	107.481	83.544	1.00	0.00	C
ATOM	439	CD2	PHE	79	110.684	107.088	83.496	1.00	0.00	C
ATOM	440	H	PHE	79	106.996	109.437	82.183	1.00	0.00	H
ATOM	441	HA	PHE	79	108.209	106.643	81.810	1.00	0.00	H
ATOM	442	1HB	PHE	79	107.558	108.258	84.363	1.00	0.00	H
ATOM	443	2HB	PHE	79	108.124	106.607	84.368	1.00	0.00	H
ATOM	444	HD1	PHE	79	109.236	109.992	84.503	1.00	0.00	H
ATOM	445	HE1	PHE	79	111.609	110.656	84.642	1.00	0.00	H
ATOM	446	HZ	PHE	79	113.384	109.073	84.006	1.00	0.00	H
ATOM	447	HE2	PHE	79	112.798	106.782	83.282	1.00	0.00	H
ATOM	448	HD2	PHE	79	110.445	106.085	83.177	1.00	0.00	H
ATOM	449	N	ALA	80	106.110	105.319	82.471	0.00	0.00	N
ATOM	450	CA	ALA	80	104.990	104.508	83.001	0.00	0.00	C
ATOM	451	C	ALA	80	105.107	104.272	84.547	0.00	0.00	C
ATOM	452	O	ALA	80	105.868	103.428	85.035	0.00	0.00	O
ATOM	453	CB	ALA	80	105.012	103.194	82.218	0.00	0.00	C
ATOM	454	H	ALA	80	107.042	104.891	82.358	0.00	0.00	H
ATOM	455	HA	ALA	80	104.026	105.000	82.765	0.00	0.00	H
ATOM	456	1HB	ALA	80	104.222	102.506	82.564	0.00	0.00	H
ATOM	457	2HB	ALA	80	104.850	103.354	81.136	0.00	0.00	H
ATOM	458	3HB	ALA	80	105.975	102.656	82.325	0.00	0.00	H
ATOM	459	N	GLY	81	104.345	105.047	85.329	1.00	0.00	N
ATOM	460	CA	GLY	81	104.419	105.001	86.811	1.00	0.00	C
ATOM	461	C	GLY	81	103.218	104.300	87.487	1.00	0.00	C
ATOM	462	O	GLY	81	102.070	104.747	87.385	1.00	0.00	O
ATOM	463	H	GLY	81	103.838	105.767	84.788	1.00	0.00	H
ATOM	464	1HA	GLY	81	105.375	104.556	87.150	1.00	0.00	H
ATOM	465	2HA	GLY	81	104.492	106.029	87.189	1.00	0.00	H
ATOM	466	N	LYS	82	103.500	103.207	88.205	0.00	0.00	N
ATOM	467	CA	LYS	82	102.483	102.410	88.951	0.00	0.00	C
ATOM	468	C	LYS	82	102.243	102.984	90.404	0.00	0.00	C
ATOM	469	O	LYS	82	103.163	102.982	91.231	0.00	0.00	O
ATOM	470	CB	LYS	82	102.939	100.916	88.804	0.00	0.00	C
ATOM	471	CG	LYS	82	102.310	99.855	89.746	0.00	0.00	C
ATOM	472	CD	LYS	82	102.506	98.366	89.344	0.00	0.00	C
ATOM	473	CE	LYS	82	103.964	97.854	89.290	0.00	0.00	C
ATOM	474	NZ	LYS	82	104.023	96.406	88.932	0.00	0.00	N
ATOM	475	1HZ	LYS	82	103.258	95.811	89.258	1.00	0.00	H
ATOM	476	2HZ	LYS	82	104.049	96.196	87.906	1.00	0.00	H
ATOM	477	3HZ	LYS	82	104.877	95.915	89.296	1.00	0.00	H
ATOM	478	H	LYS	82	104.503	102.956	88.189	0.00	0.00	H
ATOM	479	HA	LYS	82	101.518	102.463	88.412	0.00	0.00	H
ATOM	480	1HB	LYS	82	104.038	100.839	88.899	0.00	0.00	H
ATOM	481	2HB	LYS	82	102.760	100.609	87.752	0.00	0.00	H
ATOM	482	1HG	LYS	82	101.223	100.047	89.831	0.00	0.00	H
ATOM	483	2HG	LYS	82	102.711	100.010	90.766	0.00	0.00	H
ATOM	484	1HD	LYS	82	102.006	98.183	88.371	0.00	0.00	H
ATOM	485	2HD	LYS	82	101.939	97.735	90.057	0.00	0.00	H
ATOM	486	1HE	LYS	82	104.477	98.016	90.265	0.00	0.00	H
ATOM	487	2HE	LYS	82	104.562	98.441	88.556	0.00	0.00	H
ATOM	488	N	ILE	83	101.013	103.425	90.715	0.00	0.00	N

ATOM	489	CA	ILE	83	100.653	103.996	92.050	0.00	0.00	C
ATOM	490	C	ILE	83	99.997	102.861	92.910	0.00	0.00	C
ATOM	491	O	ILE	83	98.864	102.450	92.636	0.00	0.00	O
ATOM	492	CB	ILE	83	99.731	105.267	91.908	0.00	0.00	C
ATOM	493	CG2	ILE	83	99.435	105.908	93.291	0.00	0.00	C
ATOM	494	CG1	ILE	83	100.274	106.395	90.972	0.00	0.00	C
ATOM	495	CD1	ILE	83	99.796	106.303	89.513	0.00	0.00	C
ATOM	496	H	ILE	83	100.334	103.382	89.944	0.00	0.00	H
ATOM	497	HA	ILE	83	101.573	104.343	92.566	0.00	0.00	H
ATOM	498	HB	ILE	83	98.753	104.929	91.502	0.00	0.00	H
ATOM	499	1HG2	ILE	83	98.747	106.771	93.207	0.00	0.00	H
ATOM	500	2HG2	ILE	83	98.949	105.197	93.985	0.00	0.00	H
ATOM	501	3HG2	ILE	83	100.356	106.268	93.788	0.00	0.00	H
ATOM	502	1HG1	ILE	83	101.381	106.416	91.000	0.00	0.00	H
ATOM	503	2HG1	ILE	83	99.975	107.399	91.330	0.00	0.00	H
ATOM	504	1HD1	ILE	83	100.166	107.159	88.919	0.00	0.00	H
ATOM	505	2HD1	ILE	83	100.143	105.386	89.003	0.00	0.00	H
ATOM	506	3HD1	ILE	83	98.693	106.323	89.443	0.00	0.00	H
ATOM	507	N	VAL	84	100.698	102.366	93.944	1.00	0.00	N
ATOM	508	CA	VAL	84	100.244	101.190	94.755	1.00	0.00	C
ATOM	509	C	VAL	84	99.727	101.685	96.168	1.00	0.00	C
ATOM	510	O	VAL	84	100.568	101.985	97.027	1.00	0.00	O
ATOM	511	CB	VAL	84	101.388	100.119	94.872	1.00	0.00	C
ATOM	512	CG1	VAL	84	100.985	98.872	95.691	1.00	0.00	C
ATOM	513	CG2	VAL	84	101.915	99.594	93.519	1.00	0.00	C
ATOM	514	H	VAL	84	101.673	102.693	93.997	1.00	0.00	H
ATOM	515	HA	VAL	84	99.421	100.666	94.236	1.00	0.00	H
ATOM	516	HB	VAL	84	102.238	100.600	95.394	1.00	0.00	H
ATOM	517	1HG1	VAL	84	100.133	98.329	95.239	1.00	0.00	H
ATOM	518	2HG1	VAL	84	101.820	98.152	95.783	1.00	0.00	H
ATOM	519	3HG1	VAL	84	100.689	99.129	96.724	1.00	0.00	H
ATOM	520	2HG2	VAL	84	102.366	100.415	92.933	1.00	0.00	H
ATOM	521	3HG2	VAL	84	102.707	98.831	93.635	1.00	0.00	H
ATOM	522	1HG2	VAL	84	101.112	99.150	92.899	1.00	0.00	H
ATOM	523	N	PRO	85	98.394	101.783	96.473	1.00	0.00	N
ATOM	524	CA	PRO	85	97.898	102.296	97.780	1.00	0.00	C
ATOM	525	C	PRO	85	97.963	101.264	98.958	1.00	0.00	C
ATOM	526	O	PRO	85	97.609	100.091	98.822	1.00	0.00	O
ATOM	527	CB	PRO	85	96.465	102.731	97.410	1.00	0.00	C
ATOM	528	CG	PRO	85	96.034	101.769	96.303	1.00	0.00	C
ATOM	529	CD	PRO	85	97.312	101.509	95.509	1.00	0.00	C
ATOM	530	HA	PRO	85	98.468	103.206	98.052	1.00	0.00	H
ATOM	531	1HB	PRO	85	95.769	102.729	98.270	1.00	0.00	H
ATOM	532	2HB	PRO	85	96.477	103.769	97.020	1.00	0.00	H
ATOM	533	1HG	PRO	85	95.682	100.819	96.743	1.00	0.00	H
ATOM	534	2HG	PRO	85	95.213	102.164	95.675	1.00	0.00	H
ATOM	535	1HD	PRO	85	97.341	100.464	95.147	1.00	0.00	H
ATOM	536	2HD	PRO	85	97.377	102.183	94.633	1.00	0.00	H
ATOM	537	N	LYS	86	98.387	101.742	100.135	0.00	0.00	N
ATOM	538	CA	LYS	86	98.662	100.888	101.331	0.00	0.00	C
ATOM	539	C	LYS	86	97.517	99.968	101.889	0.00	0.00	C
ATOM	540	O	LYS	86	97.759	98.781	102.113	0.00	0.00	O
ATOM	541	CB	LYS	86	99.331	101.795	102.404	0.00	0.00	C
ATOM	542	CG	LYS	86	98.485	102.960	102.985	0.00	0.00	C
ATOM	543	CD	LYS	86	99.335	103.922	103.828	0.00	0.00	C
ATOM	544	CE	LYS	86	98.550	105.160	104.284	0.00	0.00	C
ATOM	545	NZ	LYS	86	99.460	106.049	105.030	0.00	0.00	N
ATOM	546	1HZ	LYS	86	98.944	106.885	105.341	1.00	0.00	H
ATOM	547	2HZ	LYS	86	99.832	105.550	105.851	1.00	0.00	H
ATOM	548	3HZ	LYS	86	100.239	106.335	104.420	1.00	0.00	H
ATOM	549	H	LYS	86	98.689	102.718	100.099	0.00	0.00	H
ATOM	550	HA	LYS	86	99.450	100.171	101.022	0.00	0.00	H
ATOM	551	1HB	LYS	86	100.269	102.203	101.974	0.00	0.00	H
ATOM	552	2HB	LYS	86	99.682	101.158	103.240	0.00	0.00	H
ATOM	553	1HG	LYS	86	97.650	102.564	103.596	0.00	0.00	H
ATOM	554	2HG	LYS	86	98.007	103.533	102.165	0.00	0.00	H
ATOM	555	1HD	LYS	86	100.211	104.244	103.232	0.00	0.00	H
ATOM	556	2HD	LYS	86	99.741	103.384	104.706	0.00	0.00	H
ATOM	557	1HE	LYS	86	97.685	104.879	104.916	0.00	0.00	H
ATOM	558	2HE	LYS	86	98.133	105.705	103.413	0.00	0.00	H
ATOM	559	N	SER	87	96.287	100.474	102.092	1.00	0.00	N
ATOM	560	CA	SER	87	95.133	99.633	102.540	1.00	0.00	C
ATOM	561	C	SER	87	94.623	98.560	101.515	1.00	0.00	C

ATOM	562	O	SER	87	94.403	97.411	101.905	1.00	0.00	O
ATOM	563	CB	SER	87	94.007	100.572	103.026	1.00	0.00	C
ATOM	564	OG	SER	87	92.956	99.832	103.653	1.00	0.00	O
ATOM	565	H	SER	87	96.215	101.475	101.887	1.00	0.00	H
ATOM	566	HA	SER	87	95.461	99.059	103.431	1.00	0.00	H
ATOM	567	1HB	SER	87	94.402	101.305	103.758	1.00	0.00	H
ATOM	568	2HB	SER	87	93.596	101.174	102.191	1.00	0.00	H
ATOM	569	HG	SER	87	92.584	99.229	102.998	1.00	0.00	H
ATOM	570	N	LEU	88	94.447	98.902	100.227	1.00	0.00	N
ATOM	571	CA	LEU	88	94.175	97.890	99.154	1.00	0.00	C
ATOM	572	C	LEU	88	95.362	96.936	98.752	1.00	0.00	C
ATOM	573	O	LEU	88	95.100	95.892	98.156	1.00	0.00	O
ATOM	574	CB	LEU	88	93.567	98.609	97.916	1.00	0.00	C
ATOM	575	CG	LEU	88	92.166	99.261	98.079	1.00	0.00	C
ATOM	576	CD1	LEU	88	91.833	100.106	96.839	1.00	0.00	C
ATOM	577	CD2	LEU	88	91.053	98.218	98.282	1.00	0.00	C
ATOM	578	H	LEU	88	94.777	99.847	100.006	1.00	0.00	H
ATOM	579	HA	LEU	88	93.404	97.191	99.529	1.00	0.00	H
ATOM	580	1HB	LEU	88	94.292	99.365	97.570	1.00	0.00	H
ATOM	581	2HB	LEU	88	93.512	97.889	97.075	1.00	0.00	H
ATOM	582	HG	LEU	88	92.179	99.938	98.956	1.00	0.00	H
ATOM	583	2HD1	LEU	88	92.580	100.904	96.672	1.00	0.00	H
ATOM	584	3HD1	LEU	88	91.798	99.496	95.915	1.00	0.00	H
ATOM	585	1HD1	LEU	88	90.851	100.605	96.935	1.00	0.00	H
ATOM	586	2HD2	LEU	88	91.004	97.492	97.449	1.00	0.00	H
ATOM	587	3HD2	LEU	88	91.192	97.637	99.211	1.00	0.00	H
ATOM	588	1HD2	LEU	88	90.055	98.690	98.359	1.00	0.00	H
ATOM	589	N	LEU	89	96.626	97.224	99.109	1.00	0.00	N
ATOM	590	CA	LEU	89	97.699	96.192	99.214	1.00	0.00	C
ATOM	591	C	LEU	89	97.562	95.227	100.455	1.00	0.00	C
ATOM	592	O	LEU	89	97.664	94.008	100.298	1.00	0.00	O
ATOM	593	CB	LEU	89	99.055	96.960	99.166	1.00	0.00	C
ATOM	594	CG	LEU	89	100.327	96.091	98.994	1.00	0.00	C
ATOM	595	CD1	LEU	89	100.467	95.560	97.558	1.00	0.00	C
ATOM	596	CD2	LEU	89	101.587	96.896	99.355	1.00	0.00	C
ATOM	597	H	LEU	89	96.766	98.189	99.426	1.00	0.00	H
ATOM	598	HA	LEU	89	97.643	95.547	98.314	1.00	0.00	H
ATOM	599	1HB	LEU	89	99.038	97.716	98.354	1.00	0.00	H
ATOM	600	2HB	LEU	89	99.142	97.561	100.093	1.00	0.00	H
ATOM	601	HG	LEU	89	100.270	95.225	99.684	1.00	0.00	H
ATOM	602	2HD1	LEU	89	99.536	95.099	97.181	1.00	0.00	H
ATOM	603	3HD1	LEU	89	100.723	96.351	96.834	1.00	0.00	H
ATOM	604	1HD1	LEU	89	101.247	94.781	97.489	1.00	0.00	H
ATOM	605	2HD2	LEU	89	101.702	97.797	98.723	1.00	0.00	H
ATOM	606	3HD2	LEU	89	101.562	97.237	100.406	1.00	0.00	H
ATOM	607	1HD2	LEU	89	102.507	96.295	99.239	1.00	0.00	H
ATOM	608	N	LEU	90	97.330	95.750	101.676	1.00	0.00	N
ATOM	609	CA	LEU	90	97.169	94.928	102.915	1.00	0.00	C
ATOM	610	C	LEU	90	95.928	93.965	102.973	1.00	0.00	C
ATOM	611	O	LEU	90	96.098	92.800	103.340	1.00	0.00	O
ATOM	612	CB	LEU	90	97.194	95.890	104.141	1.00	0.00	C
ATOM	613	CG	LEU	90	98.552	96.556	104.496	1.00	0.00	C
ATOM	614	CD1	LEU	90	98.334	97.715	105.480	1.00	0.00	C
ATOM	615	CD2	LEU	90	99.545	95.556	105.115	1.00	0.00	C
ATOM	616	H	LEU	90	97.315	96.778	101.696	1.00	0.00	H
ATOM	617	HA	LEU	90	98.046	94.258	102.994	1.00	0.00	H
ATOM	618	1HB	LEU	90	96.424	96.670	103.982	1.00	0.00	H
ATOM	619	2HB	LEU	90	96.838	95.348	105.041	1.00	0.00	H
ATOM	620	HG	LEU	90	99.004	96.976	103.574	1.00	0.00	H
ATOM	621	2HD1	LEU	90	97.669	98.489	105.053	1.00	0.00	H
ATOM	622	3HD1	LEU	90	97.880	97.378	106.432	1.00	0.00	H
ATOM	623	1HD1	LEU	90	99.284	98.222	105.733	1.00	0.00	H
ATOM	624	2HD2	LEU	90	99.137	95.070	106.021	1.00	0.00	H
ATOM	625	3HD2	LEU	90	99.817	94.752	104.408	1.00	0.00	H
ATOM	626	1HD2	LEU	90	100.488	96.050	105.410	1.00	0.00	H
ATOM	627	N	LYS	91	94.703	94.420	102.640	0.00	0.00	N
ATOM	628	CA	LYS	91	93.473	93.563	102.662	0.00	0.00	C
ATOM	629	C	LYS	91	93.508	92.243	101.787	0.00	0.00	C
ATOM	630	O	LYS	91	93.266	91.185	102.376	0.00	0.00	O
ATOM	631	CB	LYS	91	92.218	94.452	102.398	0.00	0.00	C
ATOM	632	CG	LYS	91	91.542	95.092	103.637	0.00	0.00	C
ATOM	633	CD	LYS	91	92.338	96.229	104.304	0.00	0.00	C
ATOM	634	CE	LYS	91	91.582	96.846	105.488	0.00	0.00	C

ATOM	635	NZ	LYS	91	92.386	97.929	106.087	0.00	0.00	N
ATOM	636	1HZ	LYS	91	91.873	98.339	106.881	1.00	0.00	H
ATOM	637	2HZ	LYS	91	93.283	97.549	106.419	1.00	0.00	H
ATOM	638	3HZ	LYS	91	92.562	98.657	105.380	1.00	0.00	H
ATOM	639	H	LYS	91	94.687	95.406	102.350	0.00	0.00	H
ATOM	640	HA	LYS	91	93.377	93.183	103.699	0.00	0.00	H
ATOM	641	1HB	LYS	91	91.440	93.828	101.916	0.00	0.00	H
ATOM	642	2HB	LYS	91	92.435	95.229	101.637	0.00	0.00	H
ATOM	643	1HG	LYS	91	91.314	94.304	104.382	0.00	0.00	H
ATOM	644	2HG	LYS	91	90.551	95.483	103.331	0.00	0.00	H
ATOM	645	1HD	LYS	91	92.559	97.007	103.551	0.00	0.00	H
ATOM	646	2HD	LYS	91	93.322	95.847	104.640	0.00	0.00	H
ATOM	647	1HE	LYS	91	91.361	96.077	106.256	0.00	0.00	H
ATOM	648	2HE	LYS	91	90.598	97.243	105.168	0.00	0.00	H
ATOM	649	N	PRO	92	93.817	92.198	100.453	1.00	0.00	N
ATOM	650	CA	PRO	92	94.036	90.912	99.718	1.00	0.00	C
ATOM	651	C	PRO	92	95.423	90.180	99.890	1.00	0.00	C
ATOM	652	O	PRO	92	95.793	89.369	99.038	1.00	0.00	O
ATOM	653	CB	PRO	92	93.768	91.398	98.277	1.00	0.00	C
ATOM	654	CG	PRO	92	94.319	92.824	98.235	1.00	0.00	C
ATOM	655	CD	PRO	92	93.992	93.397	99.612	1.00	0.00	C
ATOM	656	HA	PRO	92	93.260	90.170	99.994	1.00	0.00	H
ATOM	657	1HB	PRO	92	94.220	90.748	97.504	1.00	0.00	H
ATOM	658	2HB	PRO	92	92.679	91.403	98.076	1.00	0.00	H
ATOM	659	1HG	PRO	92	95.417	92.815	98.087	1.00	0.00	H
ATOM	660	2HG	PRO	92	93.897	93.431	97.411	1.00	0.00	H
ATOM	661	1HD	PRO	92	94.812	94.049	99.968	1.00	0.00	H
ATOM	662	2HD	PRO	92	93.067	94.003	99.577	1.00	0.00	H
ATOM	663	N	HIS	93	96.172	90.428	100.981	1.00	0.00	N
ATOM	664	CA	HIS	93	97.474	89.747	101.304	1.00	0.00	C
ATOM	665	C	HIS	93	98.649	89.921	100.264	1.00	0.00	C
ATOM	666	O	HIS	93	99.418	88.994	99.993	1.00	0.00	O
ATOM	667	CB	HIS	93	97.234	88.275	101.763	1.00	0.00	C
ATOM	668	CG	HIS	93	96.378	88.105	103.018	1.00	0.00	C
ATOM	669	ND1	HIS	93	96.872	88.240	104.307	1.00	0.00	N
ATOM	670	CE1	HIS	93	95.697	88.123	105.005	1.00	0.00	C
ATOM	671	NE2	HIS	93	94.519	87.915	104.337	1.00	0.00	N
ATOM	672	CD2	HIS	93	94.985	87.921	103.034	1.00	0.00	C
ATOM	673	H	HIS	93	95.706	91.058	101.647	1.00	0.00	H
ATOM	674	HA	HIS	93	97.865	90.269	102.198	1.00	0.00	H
ATOM	675	1HB	HIS	93	96.801	87.691	100.929	1.00	0.00	H
ATOM	676	2HB	HIS	93	98.208	87.786	101.958	1.00	0.00	H
ATOM	677	HE1	HIS	93	95.706	88.228	106.083	1.00	0.00	H
ATOM	678	HE2	HIS	93	93.557	87.930	104.690	1.00	0.00	H
ATOM	679	HD2	HIS	93	94.367	87.869	102.148	1.00	0.00	H
ATOM	680	N	GLN	94	98.823	91.137	99.720	0.00	0.00	N
ATOM	681	CA	GLN	94	99.797	91.412	98.619	0.00	0.00	C
ATOM	682	C	GLN	94	101.180	92.046	99.017	0.00	0.00	C
ATOM	683	O	GLN	94	102.059	92.109	98.155	0.00	0.00	O
ATOM	684	CB	GLN	94	99.060	92.295	97.574	0.00	0.00	C
ATOM	685	CG	GLN	94	97.975	91.596	96.709	0.00	0.00	C
ATOM	686	CD	GLN	94	97.355	92.477	95.614	0.00	0.00	C
ATOM	687	OE1	GLN	94	97.667	93.647	95.421	0.00	0.00	O
ATOM	688	NE2	GLN	94	96.472	91.924	94.827	0.00	0.00	N
ATOM	689	H	GLN	94	98.058	91.789	99.942	0.00	0.00	H
ATOM	690	HA	GLN	94	100.067	90.467	98.106	0.00	0.00	H
ATOM	691	1HB	GLN	94	99.805	92.722	96.876	0.00	0.00	H
ATOM	692	2HB	GLN	94	98.619	93.181	98.071	0.00	0.00	H
ATOM	693	1HG	GLN	94	97.166	91.217	97.361	0.00	0.00	H
ATOM	694	2HG	GLN	94	98.414	90.700	96.231	0.00	0.00	H
ATOM	695	1HE2	GLN	94	96.379	90.910	94.915	0.00	0.00	H
ATOM	696	2HE2	GLN	94	96.271	92.498	94.001	0.00	0.00	H
ATOM	697	N	ARG	95	101.412	92.495	100.268	1.00	0.00	N
ATOM	698	CA	ARG	95	102.691	93.151	100.696	1.00	0.00	C
ATOM	699	C	ARG	95	104.026	92.358	100.429	1.00	0.00	C
ATOM	700	O	ARG	95	104.961	92.917	99.853	1.00	0.00	O
ATOM	701	CB	ARG	95	102.495	93.590	102.174	1.00	0.00	C
ATOM	702	CG	ARG	95	103.631	94.474	102.750	1.00	0.00	C
ATOM	703	CD	ARG	95	103.389	94.848	104.218	1.00	0.00	C
ATOM	704	NE	ARG	95	104.538	95.658	104.692	1.00	0.00	N
ATOM	705	CZ	ARG	95	104.723	96.079	105.937	1.00	0.00	C
ATOM	706	NH1	ARG	95	103.907	95.845	106.921	1.00	0.00	N
ATOM	707	NH2	ARG	95	105.786	96.762	106.176	1.00	0.00	N

ATOM	708	HE	ARG	95	105.252	95.916	103.996	1.00	0.00	H
ATOM	709	H	ARG	95	100.593	92.395	100.878	1.00	0.00	H
ATOM	710	HA	ARG	95	102.788	94.078	100.097	1.00	0.00	H
ATOM	711	1HB	ARG	95	101.543	94.148	102.272	1.00	0.00	H
ATOM	712	2HB	ARG	95	102.374	92.691	102.810	1.00	0.00	H
ATOM	713	1HG	ARG	95	104.606	93.950	102.667	1.00	0.00	H
ATOM	714	2HG	ARG	95	103.748	95.395	102.145	1.00	0.00	H
ATOM	715	1HD	ARG	95	102.448	95.423	104.319	1.00	0.00	H
ATOM	716	2HD	ARG	95	103.278	93.931	104.835	1.00	0.00	H
ATOM	717	2HH1	ARG	95	103.101	95.282	106.651	1.00	0.00	H
ATOM	718	1HH1	ARG	95	104.170	96.209	107.835	1.00	0.00	H
ATOM	719	1HH2	ARG	95	106.362	96.872	105.340	1.00	0.00	H
ATOM	720	2HH2	ARG	95	105.945	97.078	107.131	1.00	0.00	H
ATOM	721	N	GLU	96	104.096	91.080	100.833	0.00	0.00	N
ATOM	722	CA	GLU	96	105.189	90.147	100.412	0.00	0.00	C
ATOM	723	C	GLU	96	104.931	89.350	99.079	0.00	0.00	C
ATOM	724	O	GLU	96	105.894	88.989	98.402	0.00	0.00	O
ATOM	725	CB	GLU	96	105.463	89.164	101.587	0.00	0.00	C
ATOM	726	CG	GLU	96	106.066	89.793	102.872	0.00	0.00	C
ATOM	727	CD	GLU	96	106.233	88.802	104.017	0.00	0.00	C
ATOM	728	OE1	GLU	96	105.377	88.590	104.869	0.00	0.00	O
ATOM	729	OE2	GLU	96	107.438	88.174	103.990	0.00	0.00	O
ATOM	730	H	GLU	96	103.250	90.754	101.306	0.00	0.00	H
ATOM	731	HA	GLU	96	106.124	90.718	100.229	0.00	0.00	H
ATOM	732	1HB	GLU	96	106.166	88.381	101.235	0.00	0.00	H
ATOM	733	2HB	GLU	96	104.534	88.612	101.832	0.00	0.00	H
ATOM	734	1HG	GLU	96	105.426	90.617	103.237	0.00	0.00	H
ATOM	735	2HG	GLU	96	107.044	90.260	102.651	0.00	0.00	H
ATOM	736	N	LYS	97	103.671	89.057	98.688	0.00	0.00	N
ATOM	737	CA	LYS	97	103.353	88.216	97.488	0.00	0.00	C
ATOM	738	C	LYS	97	103.443	88.919	96.085	0.00	0.00	C
ATOM	739	O	LYS	97	104.022	88.356	95.154	0.00	0.00	O
ATOM	740	CB	LYS	97	101.948	87.561	97.656	0.00	0.00	C
ATOM	741	CG	LYS	97	101.708	86.653	98.883	0.00	0.00	C
ATOM	742	CD	LYS	97	100.329	85.964	98.808	0.00	0.00	C
ATOM	743	CE	LYS	97	99.974	85.222	100.102	0.00	0.00	C
ATOM	744	NZ	LYS	97	98.655	84.577	99.947	0.00	0.00	N
ATOM	745	1HZ	LYS	97	98.413	84.076	100.815	1.00	0.00	H
ATOM	746	2HZ	LYS	97	97.942	85.294	99.755	1.00	0.00	H
ATOM	747	3HZ	LYS	97	98.690	83.908	99.164	1.00	0.00	H
ATOM	748	H	LYS	97	102.948	89.411	99.318	0.00	0.00	H
ATOM	749	HA	LYS	97	104.088	87.389	97.445	0.00	0.00	H
ATOM	750	1HB	LYS	97	101.171	88.351	97.642	0.00	0.00	H
ATOM	751	2HB	LYS	97	101.748	86.960	96.746	0.00	0.00	H
ATOM	752	1HG	LYS	97	102.512	85.895	98.965	0.00	0.00	H
ATOM	753	2HG	LYS	97	101.772	87.260	99.808	0.00	0.00	H
ATOM	754	1HD	LYS	97	99.549	86.725	98.598	0.00	0.00	H
ATOM	755	2HD	LYS	97	100.312	85.270	97.945	0.00	0.00	H
ATOM	756	1HE	LYS	97	100.743	84.464	100.353	0.00	0.00	H
ATOM	757	2HE	LYS	97	99.946	85.926	100.959	0.00	0.00	H
ATOM	758	N	MET	98	102.791	90.083	95.914	0.00	0.00	N
ATOM	759	CA	MET	98	102.786	90.853	94.632	0.00	0.00	C
ATOM	760	C	MET	98	103.722	92.109	94.646	0.00	0.00	C
ATOM	761	O	MET	98	104.487	92.313	93.699	0.00	0.00	O
ATOM	762	CB	MET	98	101.318	91.226	94.282	0.00	0.00	C
ATOM	763	CG	MET	98	100.475	90.087	93.674	0.00	0.00	C
ATOM	764	SD	MET	98	98.916	90.757	93.075	0.00	0.00	S
ATOM	765	CE	MET	98	98.221	89.275	92.335	0.00	0.00	C
ATOM	766	H	MET	98	102.511	90.501	96.807	0.00	0.00	H
ATOM	767	HA	MET	98	103.171	90.224	93.803	0.00	0.00	H
ATOM	768	1HB	MET	98	100.800	91.647	95.163	0.00	0.00	H
ATOM	769	2HB	MET	98	101.318	92.056	93.554	0.00	0.00	H
ATOM	770	1HG	MET	98	101.006	89.617	92.825	0.00	0.00	H
ATOM	771	2HG	MET	98	100.289	89.287	94.414	0.00	0.00	H
ATOM	772	1HE	MET	98	98.818	88.972	91.457	0.00	0.00	H
ATOM	773	2HE	MET	98	97.185	89.464	92.000	0.00	0.00	H
ATOM	774	3HE	MET	98	98.208	88.439	93.057	0.00	0.00	H
ATOM	775	N	SER	99	103.680	92.944	95.705	0.00	0.00	N
ATOM	776	CA	SER	99	104.779	93.904	95.997	0.00	0.00	C
ATOM	777	C	SER	99	106.098	93.204	96.500	0.00	0.00	C
ATOM	778	O	SER	99	106.170	91.989	96.692	0.00	0.00	O
ATOM	779	CB	SER	99	104.199	94.965	96.962	0.00	0.00	C
ATOM	780	OG	SER	99	105.102	96.061	97.138	0.00	0.00	O

ATOM	781	H	SER	99	103.120	92.555	96.475	0.00	0.00	H
ATOM	782	HA	SER	99	105.037	94.431	95.057	0.00	0.00	H
ATOM	783	1HB	SER	99	103.243	95.360	96.567	0.00	0.00	H
ATOM	784	2HB	SER	99	103.965	94.501	97.940	0.00	0.00	H
ATOM	785	HG	SER	99	104.767	96.590	97.870	0.00	0.00	H
ATOM	786	N	MET	100	107.175	93.992	96.592	1.00	0.00	N
ATOM	787	CA	MET	100	108.594	93.499	96.645	1.00	0.00	C
ATOM	788	C	MET	100	109.244	93.032	95.286	1.00	0.00	C
ATOM	789	O	MET	100	110.469	92.898	95.226	1.00	0.00	O
ATOM	790	CB	MET	100	108.921	92.578	97.861	1.00	0.00	C
ATOM	791	CG	MET	100	108.700	93.223	99.246	1.00	0.00	C
ATOM	792	SD	MET	100	109.201	92.084	100.548	1.00	0.00	S
ATOM	793	CE	MET	100	108.896	93.143	101.971	1.00	0.00	C
ATOM	794	H	MET	100	106.918	94.984	96.637	1.00	0.00	H
ATOM	795	HA	MET	100	109.184	94.413	96.850	1.00	0.00	H
ATOM	796	1HB	MET	100	108.342	91.636	97.792	1.00	0.00	H
ATOM	797	2HB	MET	100	109.979	92.253	97.800	1.00	0.00	H
ATOM	798	1HG	MET	100	109.273	94.163	99.344	1.00	0.00	H
ATOM	799	2HG	MET	100	107.633	93.478	99.390	1.00	0.00	H
ATOM	800	1HE	MET	100	109.507	94.061	101.915	1.00	0.00	H
ATOM	801	3HE	MET	100	107.830	93.435	102.019	1.00	0.00	H
ATOM	802	2HE	MET	100	109.152	92.615	102.907	1.00	0.00	H
ATOM	803	N	GLU	101	108.496	92.944	94.163	0.00	0.00	N
ATOM	804	CA	GLU	101	109.067	92.992	92.774	0.00	0.00	C
ATOM	805	C	GLU	101	110.071	94.151	92.406	0.00	0.00	C
ATOM	806	O	GLU	101	110.931	93.963	91.547	0.00	0.00	O
ATOM	807	CB	GLU	101	107.894	92.894	91.754	0.00	0.00	C
ATOM	808	CG	GLU	101	106.842	94.060	91.838	0.00	0.00	C
ATOM	809	CD	GLU	101	106.279	94.737	90.600	0.00	0.00	C
ATOM	810	OE1	GLU	101	105.843	94.086	89.632	0.00	0.00	O
ATOM	811	OE2	GLU	101	106.170	95.980	90.633	0.00	0.00	O
ATOM	812	H	GLU	101	107.491	92.835	94.351	0.00	0.00	H
ATOM	813	HA	GLU	101	109.663	92.066	92.653	0.00	0.00	H
ATOM	814	1HB	GLU	101	107.339	91.952	91.938	0.00	0.00	H
ATOM	815	2HB	GLU	101	108.294	92.806	90.725	0.00	0.00	H
ATOM	816	1HG	GLU	101	107.241	94.883	92.455	0.00	0.00	H
ATOM	817	2HG	GLU	101	105.963	93.712	92.397	0.00	0.00	H
ATOM	818	N	ILE	102	110.011	95.307	93.091	0.00	0.00	N
ATOM	819	CA	ILE	102	111.117	96.324	93.126	0.00	0.00	C
ATOM	820	C	ILE	102	112.564	95.800	93.464	0.00	0.00	C
ATOM	821	O	ILE	102	113.523	96.238	92.831	0.00	0.00	O
ATOM	822	CB	ILE	102	110.710	97.558	94.018	0.00	0.00	C
ATOM	823	CG2	ILE	102	109.536	98.355	93.396	0.00	0.00	C
ATOM	824	CG1	ILE	102	110.409	97.228	95.514	0.00	0.00	C
ATOM	825	CD1	ILE	102	110.410	98.432	96.472	0.00	0.00	C
ATOM	826	H	ILE	102	109.270	95.297	93.797	0.00	0.00	H
ATOM	827	HA	ILE	102	111.220	96.704	92.090	0.00	0.00	H
ATOM	828	HB	ILE	102	111.585	98.242	94.004	0.00	0.00	H
ATOM	829	1HG2	ILE	102	109.385	99.330	93.894	0.00	0.00	H
ATOM	830	2HG2	ILE	102	109.710	98.570	92.327	0.00	0.00	H
ATOM	831	3HG2	ILE	102	108.578	97.804	93.456	0.00	0.00	H
ATOM	832	1HG1	ILE	102	111.165	96.515	95.895	0.00	0.00	H
ATOM	833	2HG1	ILE	102	109.448	96.687	95.601	0.00	0.00	H
ATOM	834	1HD1	ILE	102	110.241	98.116	97.517	0.00	0.00	H
ATOM	835	2HD1	ILE	102	111.381	98.963	96.454	0.00	0.00	H
ATOM	836	3HD1	ILE	102	109.623	99.168	96.227	0.00	0.00	H
ATOM	837	N	SER	103	112.731	94.840	94.395	1.00	0.00	N
ATOM	838	CA	SER	103	114.010	94.078	94.548	1.00	0.00	C
ATOM	839	C	SER	103	114.407	93.084	93.393	1.00	0.00	C
ATOM	840	O	SER	103	115.580	92.714	93.302	1.00	0.00	O
ATOM	841	CB	SER	103	113.946	93.347	95.908	1.00	0.00	C
ATOM	842	OG	SER	103	115.211	92.763	96.229	1.00	0.00	O
ATOM	843	H	SER	103	111.847	94.461	94.757	1.00	0.00	H
ATOM	844	HA	SER	103	114.842	94.808	94.614	1.00	0.00	H
ATOM	845	1HB	SER	103	113.664	94.044	96.721	1.00	0.00	H
ATOM	846	2HB	SER	103	113.161	92.564	95.899	1.00	0.00	H
ATOM	847	HG	SER	103	115.563	92.369	95.418	1.00	0.00	H
ATOM	848	N	ILE	104	113.466	92.652	92.534	0.00	0.00	N
ATOM	849	CA	ILE	104	113.770	91.892	91.283	0.00	0.00	C
ATOM	850	C	ILE	104	114.234	92.901	90.167	0.00	0.00	C
ATOM	851	O	ILE	104	115.419	92.936	89.833	0.00	0.00	O
ATOM	852	CB	ILE	104	112.573	90.937	90.894	0.00	0.00	C
ATOM	853	CG2	ILE	104	112.868	90.156	89.586	0.00	0.00	C

ATOM	854	CG1	ILE	104	112.175	89.917	92.006	0.00	0.00	C
ATOM	855	CD1	ILE	104	110.818	89.209	91.806	0.00	0.00	C
ATOM	856	H	ILE	104	112.552	93.098	92.676	0.00	0.00	H
ATOM	857	HA	ILE	104	114.641	91.231	91.467	0.00	0.00	H
ATOM	858	HB	ILE	104	111.688	91.577	90.702	0.00	0.00	H
ATOM	859	1HG2	ILE	104	112.044	89.477	89.301	0.00	0.00	H
ATOM	860	2HG2	ILE	104	112.997	90.835	88.724	0.00	0.00	H
ATOM	861	3HG2	ILE	104	113.784	89.541	89.662	0.00	0.00	H
ATOM	862	1HG1	ILE	104	112.122	90.432	92.984	0.00	0.00	H
ATOM	863	2HG1	ILE	104	112.976	89.162	92.138	0.00	0.00	H
ATOM	864	1HD1	ILE	104	110.546	88.603	92.691	0.00	0.00	H
ATOM	865	2HD1	ILE	104	109.990	89.923	91.641	0.00	0.00	H
ATOM	866	3HD1	ILE	104	110.825	88.518	90.944	0.00	0.00	H
ATOM	867	N	HIS	105	113.344	93.746	89.616	1.00	0.00	N
ATOM	868	CA	HIS	105	113.695	94.702	88.517	1.00	0.00	C
ATOM	869	C	HIS	105	114.587	95.965	88.831	1.00	0.00	C
ATOM	870	O	HIS	105	114.998	96.646	87.890	1.00	0.00	O
ATOM	871	CB	HIS	105	112.403	95.005	87.708	1.00	0.00	C
ATOM	872	CG	HIS	105	111.208	95.654	88.402	1.00	0.00	C
ATOM	873	ND1	HIS	105	109.950	95.079	88.433	1.00	0.00	N
ATOM	874	CE1	HIS	105	109.254	96.094	89.029	1.00	0.00	C
ATOM	875	NE2	HIS	105	109.900	97.248	89.378	1.00	0.00	N
ATOM	876	CD2	HIS	105	111.175	96.940	88.946	1.00	0.00	C
ATOM	877	H	HIS	105	112.395	93.691	90.011	1.00	0.00	H
ATOM	878	HA	HIS	105	114.335	94.144	87.803	1.00	0.00	H
ATOM	879	1HB	HIS	105	112.660	95.634	86.835	1.00	0.00	H
ATOM	880	2HB	HIS	105	112.066	94.058	87.248	1.00	0.00	H
ATOM	881	HE1	HIS	105	108.185	95.999	89.157	1.00	0.00	H
ATOM	882	HE2	HIS	105	109.511	98.124	89.737	1.00	0.00	H
ATOM	883	HD2	HIS	105	112.024	97.602	88.960	1.00	0.00	H
ATOM	884	N	ARG	106	114.967	96.248	90.091	1.00	0.00	N
ATOM	885	CA	ARG	106	116.188	97.062	90.403	1.00	0.00	C
ATOM	886	C	ARG	106	117.561	96.302	90.234	1.00	0.00	C
ATOM	887	O	ARG	106	118.534	96.905	89.777	1.00	0.00	O
ATOM	888	CB	ARG	106	116.016	97.669	91.825	1.00	0.00	C
ATOM	889	CG	ARG	106	116.944	98.849	92.215	1.00	0.00	C
ATOM	890	CD	ARG	106	116.548	100.176	91.548	1.00	0.00	C
ATOM	891	NE	ARG	106	117.304	101.306	92.139	1.00	0.00	N
ATOM	892	CZ	ARG	106	117.196	102.573	91.754	1.00	0.00	C
ATOM	893	NH1	ARG	106	116.436	102.985	90.782	1.00	0.00	N
ATOM	894	NH2	ARG	106	117.895	103.444	92.389	1.00	0.00	N
ATOM	895	HE	ARG	106	117.960	101.093	92.904	1.00	0.00	H
ATOM	896	H	ARG	106	114.499	95.669	90.799	1.00	0.00	H
ATOM	897	HA	ARG	106	116.232	97.909	89.690	1.00	0.00	H
ATOM	898	1HB	ARG	106	114.973	98.014	91.962	1.00	0.00	H
ATOM	899	2HB	ARG	106	116.131	96.860	92.572	1.00	0.00	H
ATOM	900	1HG	ARG	106	116.907	98.977	93.315	1.00	0.00	H
ATOM	901	2HG	ARG	106	118.005	98.616	91.995	1.00	0.00	H
ATOM	902	1HD	ARG	106	116.720	100.122	90.454	1.00	0.00	H
ATOM	903	2HD	ARG	106	115.467	100.362	91.693	1.00	0.00	H
ATOM	904	2HH1	ARG	106	115.966	102.231	90.280	1.00	0.00	H
ATOM	905	1HH1	ARG	106	116.449	103.981	90.557	1.00	0.00	H
ATOM	906	1HH2	ARG	106	118.476	103.015	93.111	1.00	0.00	H
ATOM	907	2HH2	ARG	106	117.837	104.410	92.071	1.00	0.00	H
ATOM	908	N	SER	107	117.656	95.006	90.591	1.00	0.00	N
ATOM	909	CA	SER	107	118.898	94.191	90.412	1.00	0.00	C
ATOM	910	C	SER	107	119.231	93.611	88.983	1.00	0.00	C
ATOM	911	O	SER	107	120.313	93.038	88.811	1.00	0.00	O
ATOM	912	CB	SER	107	118.801	93.051	91.457	1.00	0.00	C
ATOM	913	OG	SER	107	120.020	92.306	91.515	1.00	0.00	O
ATOM	914	H	SER	107	116.758	94.573	90.835	1.00	0.00	H
ATOM	915	HA	SER	107	119.773	94.811	90.692	1.00	0.00	H
ATOM	916	1HB	SER	107	118.583	93.450	92.468	1.00	0.00	H
ATOM	917	2HB	SER	107	117.956	92.371	91.219	1.00	0.00	H
ATOM	918	HG	SER	107	120.314	92.177	90.601	1.00	0.00	H
ATOM	919	N	LEU	108	118.339	93.708	87.985	1.00	0.00	N
ATOM	920	CA	LEU	108	118.502	93.046	86.658	1.00	0.00	C
ATOM	921	C	LEU	108	119.119	94.006	85.584	1.00	0.00	C
ATOM	922	O	LEU	108	118.409	94.660	84.814	1.00	0.00	O
ATOM	923	CB	LEU	108	117.098	92.487	86.259	1.00	0.00	C
ATOM	924	CG	LEU	108	116.686	91.054	86.710	1.00	0.00	C
ATOM	925	CD1	LEU	108	117.204	90.574	88.077	1.00	0.00	C
ATOM	926	CD2	LEU	108	115.152	90.965	86.708	1.00	0.00	C

ATOM	927	H	LEU	108	117.463	94.155	88.273	1.00	0.00	H
ATOM	928	HA	LEU	108	119.184	92.174	86.733	1.00	0.00	H
ATOM	929	1HB	LEU	108	116.324	93.229	86.542	1.00	0.00	H
ATOM	930	2HB	LEU	108	117.022	92.480	85.156	1.00	0.00	H
ATOM	931	HG	LEU	108	117.076	90.334	85.960	1.00	0.00	H
ATOM	932	2HD1	LEU	108	118.307	90.517	88.100	1.00	0.00	H
ATOM	933	3HD1	LEU	108	116.898	91.239	88.903	1.00	0.00	H
ATOM	934	1HD1	LEU	108	116.842	89.558	88.321	1.00	0.00	H
ATOM	935	2HD2	LEU	108	114.700	91.680	87.419	1.00	0.00	H
ATOM	936	3HD2	LEU	108	114.728	91.191	85.712	1.00	0.00	H
ATOM	937	1HD2	LEU	108	114.791	89.961	86.993	1.00	0.00	H
ATOM	938	N	ALA	109	120.459	94.046	85.502	1.00	0.00	N
ATOM	939	CA	ALA	109	121.181	94.809	84.450	1.00	0.00	C
ATOM	940	C	ALA	109	121.276	94.026	83.092	1.00	0.00	C
ATOM	941	O	ALA	109	122.205	93.242	82.864	1.00	0.00	O
ATOM	942	CB	ALA	109	122.549	95.166	85.065	1.00	0.00	C
ATOM	943	H	ALA	109	120.937	93.517	86.238	1.00	0.00	H
ATOM	944	HA	ALA	109	120.661	95.770	84.261	1.00	0.00	H
ATOM	945	2HB	ALA	109	122.442	95.760	85.993	1.00	0.00	H
ATOM	946	3HB	ALA	109	123.147	94.269	85.313	1.00	0.00	H
ATOM	947	1HB	ALA	109	123.155	95.773	84.367	1.00	0.00	H
ATOM	948	N	HIS	110	120.281	94.224	82.211	0.00	0.00	N
ATOM	949	CA	HIS	110	120.183	93.522	80.899	0.00	0.00	C
ATOM	950	C	HIS	110	119.536	94.431	79.796	0.00	0.00	C
ATOM	951	O	HIS	110	118.774	95.359	80.081	0.00	0.00	O
ATOM	952	CB	HIS	110	119.385	92.201	81.129	0.00	0.00	C
ATOM	953	CG	HIS	110	119.470	91.154	80.018	0.00	0.00	C
ATOM	954	ND1	HIS	110	118.360	90.593	79.403	0.00	0.00	N
ATOM	955	CE1	HIS	110	118.990	89.661	78.619	0.00	0.00	C
ATOM	956	NE2	HIS	110	120.356	89.578	78.616	0.00	0.00	N
ATOM	957	CD2	HIS	110	120.651	90.545	79.559	0.00	0.00	C
ATOM	958	H	HIS	110	119.499	94.777	82.586	0.00	0.00	H
ATOM	959	HA	HIS	110	121.208	93.272	80.555	0.00	0.00	H
ATOM	960	1HB	HIS	110	118.324	92.438	81.344	0.00	0.00	H
ATOM	961	2HB	HIS	110	119.738	91.705	82.050	0.00	0.00	H
ATOM	962	HE1	HIS	110	118.402	88.948	78.058	0.00	0.00	H
ATOM	963	HE2	HIS	110	120.958	88.868	78.185	0.00	0.00	H
ATOM	964	HD2	HIS	110	121.637	90.755	79.950	0.00	0.00	H
ATOM	965	N	GLN	111	119.796	94.124	78.511	1.00	0.00	N
ATOM	966	CA	GLN	111	119.073	94.767	77.370	1.00	0.00	C
ATOM	967	C	GLN	111	117.522	94.518	77.294	1.00	0.00	C
ATOM	968	O	GLN	111	116.783	95.452	76.977	1.00	0.00	O
ATOM	969	CB	GLN	111	119.814	94.355	76.065	1.00	0.00	C
ATOM	970	CG	GLN	111	119.352	95.115	74.789	1.00	0.00	C
ATOM	971	CD	GLN	111	120.079	94.724	73.503	1.00	0.00	C
ATOM	972	OE1	GLN	111	119.676	93.832	72.768	1.00	0.00	O
ATOM	973	NE2	GLN	111	121.156	95.386	73.167	1.00	0.00	N
ATOM	974	H	GLN	111	120.352	93.273	78.391	1.00	0.00	H
ATOM	975	HA	GLN	111	119.191	95.864	77.481	1.00	0.00	H
ATOM	976	1HB	GLN	111	120.904	94.513	76.190	1.00	0.00	H
ATOM	977	2HB	GLN	111	119.695	93.264	75.901	1.00	0.00	H
ATOM	978	1HG	GLN	111	118.276	94.920	74.613	1.00	0.00	H
ATOM	979	2HG	GLN	111	119.413	96.208	74.943	1.00	0.00	H
ATOM	980	1HE2	GLN	111	121.424	96.166	73.769	1.00	0.00	H
ATOM	981	2HE2	GLN	111	121.540	95.113	72.259	1.00	0.00	H
ATOM	982	N	HIS	112	117.029	93.294	77.559	1.00	0.00	N
ATOM	983	CA	HIS	112	115.593	92.928	77.334	1.00	0.00	C
ATOM	984	C	HIS	112	114.665	93.099	78.602	1.00	0.00	C
ATOM	985	O	HIS	112	113.745	92.309	78.828	1.00	0.00	O
ATOM	986	CB	HIS	112	115.545	91.483	76.735	1.00	0.00	C
ATOM	987	CG	HIS	112	116.435	91.140	75.527	1.00	0.00	C
ATOM	988	ND1	HIS	112	116.759	92.021	74.504	1.00	0.00	N
ATOM	989	CE1	HIS	112	117.721	91.285	73.864	1.00	0.00	C
ATOM	990	NE2	HIS	112	118.030	90.033	74.311	1.00	0.00	N
ATOM	991	CD2	HIS	112	117.181	89.959	75.402	1.00	0.00	C
ATOM	992	H	HIS	112	117.723	92.612	77.883	1.00	0.00	H
ATOM	993	HA	HIS	112	115.158	93.595	76.563	1.00	0.00	H
ATOM	994	1HB	HIS	112	115.756	90.764	77.550	1.00	0.00	H
ATOM	995	2HB	HIS	112	114.502	91.264	76.442	1.00	0.00	H
ATOM	996	HE1	HIS	112	118.248	91.719	73.024	1.00	0.00	H
ATOM	997	HE2	HIS	112	118.792	89.412	74.014	1.00	0.00	H
ATOM	998	HD2	HIS	112	117.131	89.137	76.100	1.00	0.00	H
ATOM	999	N	VAL	113	114.879	94.140	79.426	1.00	0.00	N

ATOM	1000	CA	VAL	113	114.177	94.363	80.732	1.00	0.00	C
ATOM	1001	C	VAL	113	113.876	95.899	80.839	1.00	0.00	C
ATOM	1002	O	VAL	113	114.762	96.727	80.603	1.00	0.00	O
ATOM	1003	CB	VAL	113	115.031	93.822	81.942	1.00	0.00	C
ATOM	1004	CG1	VAL	113	114.422	94.136	83.330	1.00	0.00	C
ATOM	1005	CG2	VAL	113	115.264	92.290	81.916	1.00	0.00	C
ATOM	1006	H	VAL	113	115.671	94.731	79.141	1.00	0.00	H
ATOM	1007	HA	VAL	113	113.208	93.826	80.741	1.00	0.00	H
ATOM	1008	HB	VAL	113	116.025	94.314	81.899	1.00	0.00	H
ATOM	1009	1HG1	VAL	113	113.405	93.722	83.446	1.00	0.00	H
ATOM	1010	2HG1	VAL	113	115.039	93.742	84.161	1.00	0.00	H
ATOM	1011	3HG1	VAL	113	114.345	95.227	83.509	1.00	0.00	H
ATOM	1012	2HG2	VAL	113	115.809	91.975	81.008	1.00	0.00	H
ATOM	1013	3HG2	VAL	113	115.874	91.945	82.773	1.00	0.00	H
ATOM	1014	1HG2	VAL	113	114.314	91.724	81.936	1.00	0.00	H
ATOM	1015	N	VAL	114	112.642	96.296	81.208	0.00	0.00	N
ATOM	1016	CA	VAL	114	112.230	97.744	81.262	0.00	0.00	C
ATOM	1017	C	VAL	114	113.120	98.550	82.289	0.00	0.00	C
ATOM	1018	O	VAL	114	113.304	98.124	83.436	0.00	0.00	O
ATOM	1019	CB	VAL	114	110.701	97.852	81.615	0.00	0.00	C
ATOM	1020	CG1	VAL	114	110.200	99.308	81.734	0.00	0.00	C
ATOM	1021	CG2	VAL	114	109.717	97.185	80.624	0.00	0.00	C
ATOM	1022	H	VAL	114	112.016	95.535	81.503	0.00	0.00	H
ATOM	1023	HA	VAL	114	112.370	98.187	80.256	0.00	0.00	H
ATOM	1024	HB	VAL	114	110.557	97.367	82.602	0.00	0.00	H
ATOM	1025	1HG1	VAL	114	110.767	99.897	82.479	0.00	0.00	H
ATOM	1026	2HG1	VAL	114	110.258	99.866	80.780	0.00	0.00	H
ATOM	1027	3HG1	VAL	114	109.150	99.339	82.069	0.00	0.00	H
ATOM	1028	1HG2	VAL	114	109.688	97.697	79.644	0.00	0.00	H
ATOM	1029	2HG2	VAL	114	109.962	96.125	80.438	0.00	0.00	H
ATOM	1030	3HG2	VAL	114	108.678	97.192	81.006	0.00	0.00	H
ATOM	1031	N	GLY	115	113.677	99.701	81.873	1.00	0.00	N
ATOM	1032	CA	GLY	115	114.555	100.527	82.744	1.00	0.00	C
ATOM	1033	C	GLY	115	113.860	101.190	83.956	1.00	0.00	C
ATOM	1034	O	GLY	115	112.941	101.999	83.811	1.00	0.00	O
ATOM	1035	H	GLY	115	113.367	100.067	80.961	1.00	0.00	H
ATOM	1036	1HA	GLY	115	115.441	99.941	83.061	1.00	0.00	H
ATOM	1037	2HA	GLY	115	114.975	101.342	82.130	1.00	0.00	H
ATOM	1038	N	PHE	116	114.284	100.805	85.163	1.00	0.00	N
ATOM	1039	CA	PHE	116	113.653	101.270	86.423	1.00	0.00	C
ATOM	1040	C	PHE	116	114.361	102.526	87.030	1.00	0.00	C
ATOM	1041	O	PHE	116	115.506	102.470	87.485	1.00	0.00	O
ATOM	1042	CB	PHE	116	113.598	100.040	87.373	1.00	0.00	C
ATOM	1043	CG	PHE	116	112.797	100.237	88.671	1.00	0.00	C
ATOM	1044	CD1	PHE	116	111.508	100.777	88.644	1.00	0.00	C
ATOM	1045	CE1	PHE	116	110.797	100.954	89.820	1.00	0.00	C
ATOM	1046	CZ	PHE	116	111.341	100.551	91.030	1.00	0.00	C
ATOM	1047	CE2	PHE	116	112.610	99.980	91.072	1.00	0.00	C
ATOM	1048	CD2	PHE	116	113.338	99.830	89.893	1.00	0.00	C
ATOM	1049	H	PHE	116	114.915	99.996	85.144	1.00	0.00	H
ATOM	1050	HA	PHE	116	112.602	101.542	86.204	1.00	0.00	H
ATOM	1051	1HB	PHE	116	113.152	99.173	86.844	1.00	0.00	H
ATOM	1052	2HB	PHE	116	114.633	99.711	87.601	1.00	0.00	H
ATOM	1053	HD1	PHE	116	111.048	101.070	87.714	1.00	0.00	H
ATOM	1054	HE1	PHE	116	109.818	101.392	89.786	1.00	0.00	H
ATOM	1055	HZ	PHE	116	110.760	100.687	91.925	1.00	0.00	H
ATOM	1056	HE2	PHE	116	113.026	99.647	92.013	1.00	0.00	H
ATOM	1057	HD2	PHE	116	114.313	99.368	89.922	1.00	0.00	H
ATOM	1058	N	HIS	117	113.642	103.657	87.050	1.00	0.00	N
ATOM	1059	CA	HIS	117	114.145	104.947	87.595	1.00	0.00	C
ATOM	1060	C	HIS	117	114.102	105.098	89.160	1.00	0.00	C
ATOM	1061	O	HIS	117	115.055	105.637	89.731	1.00	0.00	O
ATOM	1062	CB	HIS	117	113.346	106.045	86.836	1.00	0.00	C
ATOM	1063	CG	HIS	117	113.832	107.481	87.004	1.00	0.00	C
ATOM	1064	ND1	HIS	117	113.032	108.504	87.493	1.00	0.00	N
ATOM	1065	CE1	HIS	117	113.899	109.556	87.340	1.00	0.00	C
ATOM	1066	NE2	HIS	117	115.144	109.346	86.812	1.00	0.00	N
ATOM	1067	CD2	HIS	117	115.081	107.982	86.595	1.00	0.00	C
ATOM	1068	H	HIS	117	112.668	103.548	86.734	1.00	0.00	H
ATOM	1069	HA	HIS	117	115.213	105.053	87.312	1.00	0.00	H
ATOM	1070	1HB	HIS	117	113.342	105.837	85.749	1.00	0.00	H
ATOM	1071	2HB	HIS	117	112.280	105.988	87.128	1.00	0.00	H
ATOM	1072	HE1	HIS	117	113.600	110.546	87.656	1.00	0.00	H

ATOM	1073	HE2	HIS	117	115.907	110.015	86.667	1.00	0.00	H
ATOM	1074	HD2	HIS	117	115.869	107.380	86.162	1.00	0.00	H
ATOM	1075	N	GLY	118	113.030	104.664	89.853	1.00	0.00	N
ATOM	1076	CA	GLY	118	112.920	104.847	91.324	1.00	0.00	C
ATOM	1077	C	GLY	118	111.772	104.081	92.021	1.00	0.00	C
ATOM	1078	O	GLY	118	110.634	104.043	91.544	1.00	0.00	O
ATOM	1079	H	GLY	118	112.330	104.175	89.282	1.00	0.00	H
ATOM	1080	1HA	GLY	118	113.891	104.600	91.798	1.00	0.00	H
ATOM	1081	2HA	GLY	118	112.763	105.919	91.540	1.00	0.00	H
ATOM	1082	N	PHE	119	112.086	103.527	93.199	1.00	0.00	N
ATOM	1083	CA	PHE	119	111.077	103.036	94.179	1.00	0.00	C
ATOM	1084	C	PHE	119	110.838	104.101	95.301	1.00	0.00	C
ATOM	1085	O	PHE	119	111.701	104.312	96.160	1.00	0.00	O
ATOM	1086	CB	PHE	119	111.485	101.633	94.732	1.00	0.00	C
ATOM	1087	CG	PHE	119	112.841	101.449	95.447	1.00	0.00	C
ATOM	1088	CD1	PHE	119	112.914	101.471	96.843	1.00	0.00	C
ATOM	1089	CE1	PHE	119	114.134	101.278	97.487	1.00	0.00	C
ATOM	1090	CZ	PHE	119	115.288	101.058	96.739	1.00	0.00	C
ATOM	1091	CE2	PHE	119	115.225	101.031	95.348	1.00	0.00	C
ATOM	1092	CD2	PHE	119	114.005	101.220	94.704	1.00	0.00	C
ATOM	1093	H	PHE	119	113.071	103.618	93.465	1.00	0.00	H
ATOM	1094	HA	PHE	119	110.110	102.870	93.664	1.00	0.00	H
ATOM	1095	1HB	PHE	119	110.676	101.288	95.402	1.00	0.00	H
ATOM	1096	2HB	PHE	119	111.447	100.900	93.913	1.00	0.00	H
ATOM	1097	HD1	PHE	119	112.028	101.651	97.436	1.00	0.00	H
ATOM	1098	HE1	PHE	119	114.185	101.302	98.566	1.00	0.00	H
ATOM	1099	HZ	PHE	119	116.236	100.912	97.237	1.00	0.00	H
ATOM	1100	HE2	PHE	119	116.122	100.869	94.767	1.00	0.00	H
ATOM	1101	HD2	PHE	119	113.975	101.198	93.624	1.00	0.00	H
ATOM	1102	N	PHE	120	109.682	104.788	95.304	1.00	0.00	N
ATOM	1103	CA	PHE	120	109.403	105.868	96.300	1.00	0.00	C
ATOM	1104	C	PHE	120	108.310	105.392	97.306	1.00	0.00	C
ATOM	1105	O	PHE	120	107.118	105.356	96.981	1.00	0.00	O
ATOM	1106	CB	PHE	120	109.042	107.233	95.639	1.00	0.00	C
ATOM	1107	CG	PHE	120	109.881	107.724	94.442	1.00	0.00	C
ATOM	1108	CD1	PHE	120	109.235	108.097	93.260	1.00	0.00	C
ATOM	1109	CE1	PHE	120	109.976	108.511	92.159	1.00	0.00	C
ATOM	1110	CZ	PHE	120	111.364	108.551	92.223	1.00	0.00	C
ATOM	1111	CE2	PHE	120	112.017	108.195	93.399	1.00	0.00	C
ATOM	1112	CD2	PHE	120	111.279	107.789	94.510	1.00	0.00	C
ATOM	1113	H	PHE	120	109.077	104.606	94.491	1.00	0.00	H
ATOM	1114	HA	PHE	120	110.320	106.093	96.884	1.00	0.00	H
ATOM	1115	1HB	PHE	120	107.971	107.235	95.375	1.00	0.00	H
ATOM	1116	2HB	PHE	120	109.108	108.011	96.421	1.00	0.00	H
ATOM	1117	HD1	PHE	120	108.157	108.067	93.183	1.00	0.00	H
ATOM	1118	HE1	PHE	120	109.473	108.812	91.255	1.00	0.00	H
ATOM	1119	HZ	PHE	120	111.928	108.856	91.355	1.00	0.00	H
ATOM	1120	HE2	PHE	120	113.096	108.229	93.448	1.00	0.00	H
ATOM	1121	HD2	PHE	120	111.798	107.499	95.411	1.00	0.00	H
ATOM	1122	N	GLU	121	108.716	105.034	98.534	1.00	0.00	N
ATOM	1123	CA	GLU	121	107.772	104.624	99.617	1.00	0.00	C
ATOM	1124	C	GLU	121	107.252	105.878	100.408	1.00	0.00	C
ATOM	1125	O	GLU	121	107.704	106.199	101.511	1.00	0.00	O
ATOM	1126	CB	GLU	121	108.493	103.563	100.497	1.00	0.00	C
ATOM	1127	CG	GLU	121	108.826	102.219	99.790	1.00	0.00	C
ATOM	1128	CD	GLU	121	109.594	101.222	100.647	1.00	0.00	C
ATOM	1129	OE1	GLU	121	110.803	101.042	100.568	1.00	0.00	O
ATOM	1130	OE2	GLU	121	108.785	100.544	101.503	1.00	0.00	O
ATOM	1131	H	GLU	121	109.733	105.042	98.666	1.00	0.00	H
ATOM	1132	HA	GLU	121	106.880	104.122	99.186	1.00	0.00	H
ATOM	1133	1HB	GLU	121	109.416	104.005	100.925	1.00	0.00	H
ATOM	1134	2HB	GLU	121	107.857	103.346	101.378	1.00	0.00	H
ATOM	1135	1HG	GLU	121	107.903	101.733	99.430	1.00	0.00	H
ATOM	1136	2HG	GLU	121	109.430	102.401	98.880	1.00	0.00	H
ATOM	1137	N	ASP	122	106.311	106.615	99.798	1.00	0.00	N
ATOM	1138	CA	ASP	122	105.920	107.981	100.241	1.00	0.00	C
ATOM	1139	C	ASP	122	104.687	107.918	101.192	1.00	0.00	C
ATOM	1140	O	ASP	122	103.546	107.784	100.747	1.00	0.00	O
ATOM	1141	CB	ASP	122	105.642	108.842	98.977	1.00	0.00	C
ATOM	1142	CG	ASP	122	106.847	109.209	98.112	1.00	0.00	C
ATOM	1143	OD1	ASP	122	108.010	109.218	98.500	1.00	0.00	O
ATOM	1144	OD2	ASP	122	106.480	109.557	96.851	1.00	0.00	O
ATOM	1145	H	ASP	122	105.914	106.174	98.957	1.00	0.00	H

ATOM	1146	HA	ASP	122	106.761	108.465	100.784	1.00	0.00	H
ATOM	1147	1HB	ASP	122	104.884	108.341	98.348	1.00	0.00	H
ATOM	1148	2HB	ASP	122	105.175	109.796	99.277	1.00	0.00	H
ATOM	1149	N	ASN	123	104.925	107.982	102.515	1.00	0.00	N
ATOM	1150	CA	ASN	123	103.886	107.675	103.557	1.00	0.00	C
ATOM	1151	C	ASN	123	103.339	106.194	103.514	1.00	0.00	C
ATOM	1152	O	ASN	123	102.127	105.962	103.542	1.00	0.00	O
ATOM	1153	CB	ASN	123	102.752	108.748	103.604	1.00	0.00	C
ATOM	1154	CG	ASN	123	103.189	110.195	103.819	1.00	0.00	C
ATOM	1155	OD1	ASN	123	103.643	110.586	104.886	1.00	0.00	O
ATOM	1156	ND2	ASN	123	103.070	111.034	102.823	1.00	0.00	N
ATOM	1157	H	ASN	123	105.924	108.049	102.740	1.00	0.00	H
ATOM	1158	HA	ASN	123	104.400	107.744	104.536	1.00	0.00	H
ATOM	1159	1HB	ASN	123	102.123	108.658	102.700	1.00	0.00	H
ATOM	1160	2HB	ASN	123	102.063	108.508	104.435	1.00	0.00	H
ATOM	1161	1HD2	ASN	123	103.425	111.971	103.025	1.00	0.00	H
ATOM	1162	2HD2	ASN	123	102.787	110.631	101.927	1.00	0.00	H
ATOM	1163	N	ASP	124	104.237	105.188	103.438	1.00	0.00	N
ATOM	1164	CA	ASP	124	103.882	103.736	103.266	1.00	0.00	C
ATOM	1165	C	ASP	124	103.351	103.261	101.859	1.00	0.00	C
ATOM	1166	O	ASP	124	103.606	102.112	101.488	1.00	0.00	O
ATOM	1167	CB	ASP	124	103.058	103.142	104.444	1.00	0.00	C
ATOM	1168	CG	ASP	124	103.715	103.228	105.818	1.00	0.00	C
ATOM	1169	OD1	ASP	124	104.749	102.645	106.119	1.00	0.00	O
ATOM	1170	OD2	ASP	124	103.021	104.022	106.677	1.00	0.00	O
ATOM	1171	H	ASP	124	105.196	105.526	103.305	1.00	0.00	H
ATOM	1172	HA	ASP	124	104.861	103.217	103.318	1.00	0.00	H
ATOM	1173	1HB	ASP	124	102.065	103.615	104.486	1.00	0.00	H
ATOM	1174	2HB	ASP	124	102.859	102.072	104.258	1.00	0.00	H
ATOM	1175	N	PHE	125	102.625	104.082	101.077	1.00	0.00	N
ATOM	1176	CA	PHE	125	102.218	103.745	99.679	1.00	0.00	C
ATOM	1177	C	PHE	125	103.367	103.892	98.614	1.00	0.00	C
ATOM	1178	O	PHE	125	104.244	104.757	98.716	1.00	0.00	O
ATOM	1179	CB	PHE	125	100.901	104.492	99.325	1.00	0.00	C
ATOM	1180	CG	PHE	125	100.837	106.028	99.414	1.00	0.00	C
ATOM	1181	CD1	PHE	125	100.333	106.635	100.570	1.00	0.00	C
ATOM	1182	CE1	PHE	125	100.190	108.019	100.631	1.00	0.00	C
ATOM	1183	CZ	PHE	125	100.550	108.805	99.539	1.00	0.00	C
ATOM	1184	CE2	PHE	125	101.055	108.208	98.386	1.00	0.00	C
ATOM	1185	CD2	PHE	125	101.200	106.824	98.323	1.00	0.00	C
ATOM	1186	H	PHE	125	102.548	105.039	101.444	1.00	0.00	H
ATOM	1187	HA	PHE	125	101.938	102.672	99.674	1.00	0.00	H
ATOM	1188	1HB	PHE	125	100.599	104.191	98.304	1.00	0.00	H
ATOM	1189	2HB	PHE	125	100.100	104.073	99.960	1.00	0.00	H
ATOM	1190	HD1	PHE	125	100.052	106.040	101.426	1.00	0.00	H
ATOM	1191	HE1	PHE	125	99.803	108.482	101.528	1.00	0.00	H
ATOM	1192	HZ	PHE	125	100.441	109.878	99.588	1.00	0.00	H
ATOM	1193	HE2	PHE	125	101.326	108.821	97.541	1.00	0.00	H
ATOM	1194	HD2	PHE	125	101.594	106.371	97.423	1.00	0.00	H
ATOM	1195	N	VAL	126	103.404	102.985	97.623	1.00	0.00	N
ATOM	1196	CA	VAL	126	104.648	102.689	96.843	1.00	0.00	C
ATOM	1197	C	VAL	126	104.499	103.180	95.362	1.00	0.00	C
ATOM	1198	O	VAL	126	103.635	102.708	94.614	1.00	0.00	O
ATOM	1199	CB	VAL	126	105.031	101.163	96.936	1.00	0.00	C
ATOM	1200	CG1	VAL	126	106.404	100.850	96.290	1.00	0.00	C
ATOM	1201	CG2	VAL	126	105.081	100.582	98.371	1.00	0.00	C
ATOM	1202	H	VAL	126	102.554	102.412	97.532	1.00	0.00	H
ATOM	1203	HA	VAL	126	105.504	103.229	97.296	1.00	0.00	H
ATOM	1204	HB	VAL	126	104.264	100.587	96.380	1.00	0.00	H
ATOM	1205	1HG1	VAL	126	107.235	101.379	96.795	1.00	0.00	H
ATOM	1206	2HG1	VAL	126	106.641	99.769	96.314	1.00	0.00	H
ATOM	1207	3HG1	VAL	126	106.439	101.147	95.225	1.00	0.00	H
ATOM	1208	2HG2	VAL	126	104.092	100.624	98.866	1.00	0.00	H
ATOM	1209	3HG2	VAL	126	105.391	99.521	98.392	1.00	0.00	H
ATOM	1210	1HG2	VAL	126	105.773	101.142	99.025	1.00	0.00	H
ATOM	1211	N	PHE	127	105.383	104.087	94.921	1.00	0.00	N
ATOM	1212	CA	PHE	127	105.474	104.515	93.496	1.00	0.00	C
ATOM	1213	C	PHE	127	106.590	103.719	92.746	1.00	0.00	C
ATOM	1214	O	PHE	127	107.765	103.756	93.129	1.00	0.00	O
ATOM	1215	CB	PHE	127	105.762	106.036	93.415	1.00	0.00	C
ATOM	1216	CG	PHE	127	104.615	106.959	93.846	1.00	0.00	C
ATOM	1217	CD1	PHE	127	104.543	107.434	95.159	1.00	0.00	C
ATOM	1218	CE1	PHE	127	103.508	108.284	95.539	1.00	0.00	C

ATOM	1219	CZ	PHE	127	102.537	108.658	94.615	1.00	0.00	C
ATOM	1220	CE2	PHE	127	102.603	108.186	93.306	1.00	0.00	C
ATOM	1221	CD2	PHE	127	103.636	107.337	92.922	1.00	0.00	C
ATOM	1222	H	PHE	127	105.994	104.480	95.651	1.00	0.00	H
ATOM	1223	HA	PHE	127	104.504	104.346	92.983	1.00	0.00	H
ATOM	1224	1HB	PHE	127	106.677	106.262	93.988	1.00	0.00	H
ATOM	1225	2HB	PHE	127	106.045	106.300	92.376	1.00	0.00	H
ATOM	1226	HD1	PHE	127	105.287	107.144	95.888	1.00	0.00	H
ATOM	1227	HE1	PHE	127	103.464	108.655	96.551	1.00	0.00	H
ATOM	1228	HZ	PHE	127	101.733	109.317	94.911	1.00	0.00	H
ATOM	1229	HE2	PHE	127	101.855	108.475	92.583	1.00	0.00	H
ATOM	1230	HD2	PHE	127	103.676	106.974	91.905	1.00	0.00	H
ATOM	1231	N	VAL	128	106.219	103.025	91.663	1.00	0.00	N
ATOM	1232	CA	VAL	128	107.158	102.171	90.872	1.00	0.00	C
ATOM	1233	C	VAL	128	107.331	102.863	89.474	1.00	0.00	C
ATOM	1234	O	VAL	128	106.446	102.756	88.615	1.00	0.00	O
ATOM	1235	CB	VAL	128	106.594	100.701	90.814	1.00	0.00	C
ATOM	1236	CG1	VAL	128	107.465	99.721	89.999	1.00	0.00	C
ATOM	1237	CG2	VAL	128	106.366	100.039	92.194	1.00	0.00	C
ATOM	1238	H	VAL	128	105.201	103.006	91.501	1.00	0.00	H
ATOM	1239	HA	VAL	128	108.153	102.117	91.363	1.00	0.00	H
ATOM	1240	HB	VAL	128	105.612	100.748	90.316	1.00	0.00	H
ATOM	1241	1HG1	VAL	128	107.653	100.079	88.969	1.00	0.00	H
ATOM	1242	2HG1	VAL	128	108.447	99.557	90.475	1.00	0.00	H
ATOM	1243	3HG1	VAL	128	106.997	98.722	89.899	1.00	0.00	H
ATOM	1244	2HG2	VAL	128	105.597	100.584	92.771	1.00	0.00	H
ATOM	1245	3HG2	VAL	128	106.020	98.990	92.117	1.00	0.00	H
ATOM	1246	1HG2	VAL	128	107.283	100.036	92.811	1.00	0.00	H
ATOM	1247	N	VAL	129	108.436	103.608	89.266	0.00	0.00	N
ATOM	1248	CA	VAL	129	108.635	104.444	88.036	0.00	0.00	C
ATOM	1249	C	VAL	129	109.469	103.667	86.957	0.00	0.00	C
ATOM	1250	O	VAL	129	110.682	103.484	87.095	0.00	0.00	O
ATOM	1251	CB	VAL	129	109.234	105.842	88.417	0.00	0.00	C
ATOM	1252	CG1	VAL	129	109.436	106.777	87.201	0.00	0.00	C
ATOM	1253	CG2	VAL	129	108.356	106.644	89.410	0.00	0.00	C
ATOM	1254	H	VAL	129	109.032	103.732	90.098	0.00	0.00	H
ATOM	1255	HA	VAL	129	107.648	104.677	87.586	0.00	0.00	H
ATOM	1256	HB	VAL	129	110.228	105.683	88.887	0.00	0.00	H
ATOM	1257	1HG1	VAL	129	109.949	107.717	87.483	0.00	0.00	H
ATOM	1258	2HG1	VAL	129	110.064	106.319	86.415	0.00	0.00	H
ATOM	1259	3HG1	VAL	129	108.480	107.059	86.723	0.00	0.00	H
ATOM	1260	1HG2	VAL	129	108.744	107.665	89.571	0.00	0.00	H
ATOM	1261	2HG2	VAL	129	107.313	106.749	89.057	0.00	0.00	H
ATOM	1262	3HG2	VAL	129	108.321	106.161	90.404	0.00	0.00	H
ATOM	1263	N	LEU	130	108.799	103.224	85.886	1.00	0.00	N
ATOM	1264	CA	LEU	130	109.415	102.478	84.746	1.00	0.00	C
ATOM	1265	C	LEU	130	109.327	103.300	83.403	1.00	0.00	C
ATOM	1266	O	LEU	130	108.558	104.257	83.303	1.00	0.00	O
ATOM	1267	CB	LEU	130	108.620	101.133	84.676	1.00	0.00	C
ATOM	1268	CG	LEU	130	108.913	100.080	85.784	1.00	0.00	C
ATOM	1269	CD1	LEU	130	107.776	99.055	85.901	1.00	0.00	C
ATOM	1270	CD2	LEU	130	110.226	99.320	85.529	1.00	0.00	C
ATOM	1271	H	LEU	130	107.802	103.474	85.837	1.00	0.00	H
ATOM	1272	HA	LEU	130	110.488	102.267	84.925	1.00	0.00	H
ATOM	1273	1HB	LEU	130	107.535	101.361	84.647	1.00	0.00	H
ATOM	1274	2HB	LEU	130	108.787	100.665	83.694	1.00	0.00	H
ATOM	1275	HG	LEU	130	108.983	100.603	86.758	1.00	0.00	H
ATOM	1276	2HD1	LEU	130	107.947	98.341	86.729	1.00	0.00	H
ATOM	1277	3HD1	LEU	130	106.801	99.541	86.090	1.00	0.00	H
ATOM	1278	1HD1	LEU	130	107.665	98.457	84.978	1.00	0.00	H
ATOM	1279	2HD2	LEU	130	110.487	98.655	86.373	1.00	0.00	H
ATOM	1280	3HD2	LEU	130	110.172	98.685	84.626	1.00	0.00	H
ATOM	1281	1HD2	LEU	130	111.082	100.001	85.379	1.00	0.00	H
ATOM	1282	N	GLU	131	110.080	102.933	82.351	0.00	0.00	N
ATOM	1283	CA	GLU	131	110.020	103.629	81.016	0.00	0.00	C
ATOM	1284	C	GLU	131	108.628	103.573	80.266	0.00	0.00	C
ATOM	1285	O	GLU	131	107.847	102.634	80.440	0.00	0.00	O
ATOM	1286	CB	GLU	131	111.158	103.061	80.122	0.00	0.00	C
ATOM	1287	CG	GLU	131	112.609	103.393	80.570	0.00	0.00	C
ATOM	1288	CD	GLU	131	113.670	102.993	79.570	0.00	0.00	C
ATOM	1289	OE1	GLU	131	114.111	101.850	79.583	0.00	0.00	O
ATOM	1290	OE2	GLU	131	114.051	103.935	78.666	0.00	0.00	O
ATOM	1291	H	GLU	131	110.871	102.320	82.581	0.00	0.00	H

ATOM	1292	HA	GLU	131	110.247	104.702	81.185	0.00	0.00	H
ATOM	1293	1HB	GLU	131	111.036	103.469	79.097	0.00	0.00	H
ATOM	1294	2HB	GLU	131	111.040	101.969	79.995	0.00	0.00	H
ATOM	1295	1HG	GLU	131	112.861	102.929	81.533	0.00	0.00	H
ATOM	1296	2HG	GLU	131	112.727	104.481	80.717	0.00	0.00	H
ATOM	1297	N	LEU	132	108.277	104.581	79.443	1.00	0.00	N
ATOM	1298	CA	LEU	132	106.903	104.705	78.848	1.00	0.00	C
ATOM	1299	C	LEU	132	106.653	103.852	77.552	1.00	0.00	C
ATOM	1300	O	LEU	132	106.574	104.373	76.440	1.00	0.00	O
ATOM	1301	CB	LEU	132	106.596	106.229	78.718	1.00	0.00	C
ATOM	1302	CG	LEU	132	105.145	106.739	78.479	1.00	0.00	C
ATOM	1303	CD1	LEU	132	104.708	106.724	77.008	1.00	0.00	C
ATOM	1304	CD2	LEU	132	104.071	106.043	79.333	1.00	0.00	C
ATOM	1305	H	LEU	132	109.018	105.267	79.254	1.00	0.00	H
ATOM	1306	HA	LEU	132	106.180	104.329	79.594	1.00	0.00	H
ATOM	1307	1HB	LEU	132	106.924	106.718	79.651	1.00	0.00	H
ATOM	1308	2HB	LEU	132	107.268	106.664	77.950	1.00	0.00	H
ATOM	1309	HG	LEU	132	105.158	107.808	78.772	1.00	0.00	H
ATOM	1310	2HD1	LEU	132	103.786	107.316	76.851	1.00	0.00	H
ATOM	1311	3HD1	LEU	132	105.484	107.156	76.347	1.00	0.00	H
ATOM	1312	1HD1	LEU	132	104.505	105.704	76.637	1.00	0.00	H
ATOM	1313	2HD2	LEU	132	103.075	106.495	79.174	1.00	0.00	H
ATOM	1314	3HD2	LEU	132	103.980	104.969	79.087	1.00	0.00	H
ATOM	1315	1HD2	LEU	132	104.296	106.123	80.410	1.00	0.00	H
ATOM	1316	N	CYS	133	106.472	102.527	77.702	1.00	0.00	N
ATOM	1317	CA	CYS	133	106.426	101.589	76.542	1.00	0.00	C
ATOM	1318	C	CYS	133	105.037	100.892	76.285	1.00	0.00	C
ATOM	1319	O	CYS	133	104.198	100.720	77.177	1.00	0.00	O
ATOM	1320	CB	CYS	133	107.598	100.603	76.742	1.00	0.00	C
ATOM	1321	SG	CYS	133	109.201	101.492	76.858	1.00	0.00	S
ATOM	1322	H	CYS	133	106.732	102.222	78.648	1.00	0.00	H
ATOM	1323	HA	CYS	133	106.666	102.141	75.607	1.00	0.00	H
ATOM	1324	1HB	CYS	133	107.458	99.988	77.648	1.00	0.00	H
ATOM	1325	2HB	CYS	133	107.663	99.900	75.893	1.00	0.00	H
ATOM	1326	HG	CYS	133	109.042	102.358	75.852	1.00	0.00	H
ATOM	1327	N	ARG	134	104.775	100.465	75.033	1.00	0.00	N
ATOM	1328	CA	ARG	134	103.490	99.798	74.659	1.00	0.00	C
ATOM	1329	C	ARG	134	103.590	98.225	74.735	1.00	0.00	C
ATOM	1330	O	ARG	134	104.065	97.571	73.813	1.00	0.00	O
ATOM	1331	CB	ARG	134	103.084	100.221	73.216	1.00	0.00	C
ATOM	1332	CG	ARG	134	102.443	101.619	73.038	1.00	0.00	C
ATOM	1333	CD	ARG	134	101.887	101.772	71.607	1.00	0.00	C
ATOM	1334	NE	ARG	134	101.161	103.064	71.452	1.00	0.00	N
ATOM	1335	CZ	ARG	134	100.461	103.419	70.376	1.00	0.00	C
ATOM	1336	NH1	ARG	134	100.385	102.699	69.293	1.00	0.00	N
ATOM	1337	NH2	ARG	134	99.837	104.556	70.389	1.00	0.00	N
ATOM	1338	HE	ARG	134	101.171	103.752	72.213	1.00	0.00	H
ATOM	1339	H	ARG	134	105.593	100.514	74.405	1.00	0.00	H
ATOM	1340	HA	ARG	134	102.674	100.125	75.335	1.00	0.00	H
ATOM	1341	1HB	ARG	134	103.960	100.113	72.542	1.00	0.00	H
ATOM	1342	2HB	ARG	134	102.359	99.472	72.836	1.00	0.00	H
ATOM	1343	1HG	ARG	134	101.637	101.756	73.785	1.00	0.00	H
ATOM	1344	2HG	ARG	134	103.197	102.403	73.263	1.00	0.00	H
ATOM	1345	1HD	ARG	134	102.727	101.701	70.882	1.00	0.00	H
ATOM	1346	2HD	ARG	134	101.205	100.921	71.383	1.00	0.00	H
ATOM	1347	2HH1	ARG	134	100.927	101.836	69.356	1.00	0.00	H
ATOM	1348	1HH1	ARG	134	99.983	103.155	68.477	1.00	0.00	H
ATOM	1349	1HH2	ARG	134	99.920	105.082	71.261	1.00	0.00	H
ATOM	1350	2HH2	ARG	134	99.221	104.761	69.596	1.00	0.00	H
ATOM	1351	N	ARG	135	103.087	97.624	75.813	1.00	0.00	N
ATOM	1352	CA	ARG	135	102.444	96.259	75.882	1.00	0.00	C
ATOM	1353	C	ARG	135	102.227	95.298	74.626	1.00	0.00	C
ATOM	1354	O	ARG	135	102.193	95.768	73.496	1.00	0.00	O
ATOM	1355	CB	ARG	135	101.170	96.500	76.763	1.00	0.00	C
ATOM	1356	CG	ARG	135	100.249	97.756	76.533	1.00	0.00	C
ATOM	1357	CD	ARG	135	99.239	98.054	77.662	1.00	0.00	C
ATOM	1358	NE	ARG	135	98.236	96.968	77.722	1.00	0.00	N
ATOM	1359	CZ	ARG	135	98.273	96.032	78.641	1.00	0.00	C
ATOM	1360	NH1	ARG	135	98.483	96.230	79.894	1.00	0.00	N
ATOM	1361	NH2	ARG	135	98.048	94.829	78.294	1.00	0.00	N
ATOM	1362	HE	ARG	135	97.982	96.480	76.853	1.00	0.00	H
ATOM	1363	H	ARG	135	102.981	98.280	76.595	1.00	0.00	H
ATOM	1364	HA	ARG	135	103.127	95.662	76.520	1.00	0.00	H

ATOM	1365	1HB	ARG	135	100.547	95.585	76.749	1.00	0.00	H
ATOM	1366	2HB	ARG	135	101.503	96.524	77.819	1.00	0.00	H
ATOM	1367	1HG	ARG	135	100.861	98.670	76.445	1.00	0.00	H
ATOM	1368	2HG	ARG	135	99.741	97.682	75.554	1.00	0.00	H
ATOM	1369	1HD	ARG	135	99.775	98.187	78.627	1.00	0.00	H
ATOM	1370	2HD	ARG	135	98.722	99.018	77.487	1.00	0.00	H
ATOM	1371	2HH1	ARG	135	97.841	96.966	80.275	1.00	0.00	H
ATOM	1372	1HH1	ARG	135	98.325	95.288	80.351	1.00	0.00	H
ATOM	1373	1HH2	ARG	135	97.606	94.599	77.401	1.00	0.00	H
ATOM	1374	2HH2	ARG	135	97.832	94.231	79.153	1.00	0.00	H
ATOM	1375	N	ARG	136	102.093	93.951	74.777	1.00	0.00	N
ATOM	1376	CA	ARG	136	102.057	92.967	73.624	1.00	0.00	C
ATOM	1377	C	ARG	136	100.688	92.376	73.061	1.00	0.00	C
ATOM	1378	O	ARG	136	100.739	91.506	72.193	1.00	0.00	O
ATOM	1379	CB	ARG	136	103.087	91.811	73.900	1.00	0.00	C
ATOM	1380	CG	ARG	136	104.158	91.580	72.810	1.00	0.00	C
ATOM	1381	CD	ARG	136	105.251	92.657	72.832	1.00	0.00	C
ATOM	1382	NE	ARG	136	106.206	92.383	71.732	1.00	0.00	N
ATOM	1383	CZ	ARG	136	107.389	92.960	71.582	1.00	0.00	C
ATOM	1384	NH1	ARG	136	107.878	93.831	72.403	1.00	0.00	N
ATOM	1385	NH2	ARG	136	108.094	92.643	70.557	1.00	0.00	N
ATOM	1386	HE	ARG	136	105.927	91.687	71.026	1.00	0.00	H
ATOM	1387	H	ARG	136	102.248	93.616	75.740	1.00	0.00	H
ATOM	1388	HA	ARG	136	102.443	93.480	72.718	1.00	0.00	H
ATOM	1389	1HB	ARG	136	103.582	91.925	74.880	1.00	0.00	H
ATOM	1390	2HB	ARG	136	102.546	90.859	74.040	1.00	0.00	H
ATOM	1391	1HG	ARG	136	104.633	90.591	72.959	1.00	0.00	H
ATOM	1392	2HG	ARG	136	103.686	91.522	71.809	1.00	0.00	H
ATOM	1393	1HD	ARG	136	104.817	93.671	72.717	1.00	0.00	H
ATOM	1394	2HD	ARG	136	105.766	92.652	73.815	1.00	0.00	H
ATOM	1395	2HH1	ARG	136	107.240	94.080	73.160	1.00	0.00	H
ATOM	1396	1HH1	ARG	136	108.786	94.233	72.170	1.00	0.00	H
ATOM	1397	1HH2	ARG	136	107.610	91.983	69.942	1.00	0.00	H
ATOM	1398	2HH2	ARG	136	108.989	93.111	70.433	1.00	0.00	H
ATOM	1399	N	SER	137	99.408	92.748	73.311	1.00	0.00	N
ATOM	1400	CA	SER	137	98.894	93.583	74.450	1.00	0.00	C
ATOM	1401	C	SER	137	98.599	95.136	74.259	1.00	0.00	C
ATOM	1402	O	SER	137	98.196	95.769	75.225	1.00	0.00	O
ATOM	1403	CB	SER	137	97.668	92.796	75.047	1.00	0.00	C
ATOM	1404	OG	SER	137	96.959	93.495	76.093	1.00	0.00	O
ATOM	1405	H	SER	137	98.778	92.393	72.582	1.00	0.00	H
ATOM	1406	HA	SER	137	99.623	93.559	75.279	1.00	0.00	H
ATOM	1407	1HB	SER	137	96.937	92.555	74.252	1.00	0.00	H
ATOM	1408	2HB	SER	137	97.996	91.822	75.453	1.00	0.00	H
ATOM	1409	HG	SER	137	96.783	92.949	76.949	1.00	0.00	H
ATOM	1410	N	LEU	138	98.732	96.006	73.240	1.00	0.00	N
ATOM	1411	CA	LEU	138	98.781	95.723	71.777	1.00	0.00	C
ATOM	1412	C	LEU	138	97.517	94.909	71.295	1.00	0.00	C
ATOM	1413	O	LEU	138	97.528	93.692	71.106	1.00	0.00	O
ATOM	1414	CB	LEU	138	100.246	95.409	71.362	1.00	0.00	C
ATOM	1415	CG	LEU	138	100.687	95.099	69.916	1.00	0.00	C
ATOM	1416	CD1	LEU	138	102.198	94.813	69.905	1.00	0.00	C
ATOM	1417	CD2	LEU	138	100.015	93.877	69.283	1.00	0.00	C
ATOM	1418	H	LEU	138	98.550	96.940	73.620	1.00	0.00	H
ATOM	1419	HA	LEU	138	98.653	96.705	71.281	1.00	0.00	H
ATOM	1420	1HB	LEU	138	100.846	96.286	71.679	1.00	0.00	H
ATOM	1421	2HB	LEU	138	100.635	94.628	72.003	1.00	0.00	H
ATOM	1422	HG	LEU	138	100.492	95.999	69.305	1.00	0.00	H
ATOM	1423	2HD1	LEU	138	102.762	95.565	70.484	1.00	0.00	H
ATOM	1424	3HD1	LEU	138	102.447	93.835	70.362	1.00	0.00	H
ATOM	1425	1HD1	LEU	138	102.610	94.808	68.881	1.00	0.00	H
ATOM	1426	2HD2	LEU	138	100.082	92.981	69.930	1.00	0.00	H
ATOM	1427	3HD2	LEU	138	98.945	94.055	69.092	1.00	0.00	H
ATOM	1428	1HD2	LEU	138	100.466	93.612	68.310	1.00	0.00	H
ATOM	1429	N	LEU	139	96.395	95.647	71.172	1.00	0.00	N
ATOM	1430	CA	LEU	139	95.028	95.086	71.001	1.00	0.00	C
ATOM	1431	C	LEU	139	94.092	95.753	69.895	1.00	0.00	C
ATOM	1432	O	LEU	139	92.912	95.417	69.861	1.00	0.00	O
ATOM	1433	CB	LEU	139	94.384	95.134	72.442	1.00	0.00	C
ATOM	1434	CG	LEU	139	93.658	93.861	72.954	1.00	0.00	C
ATOM	1435	CD1	LEU	139	93.431	93.946	74.475	1.00	0.00	C
ATOM	1436	CD2	LEU	139	92.298	93.624	72.287	1.00	0.00	C
ATOM	1437	H	LEU	139	96.525	96.607	71.496	1.00	0.00	H

ATOM	1438	HA	LEU	139	95.105	94.027	70.683	1.00	0.00	H
ATOM	1439	1HB	LEU	139	95.156	95.360	73.209	1.00	0.00	H
ATOM	1440	2HB	LEU	139	93.707	96.006	72.523	1.00	0.00	H
ATOM	1441	HG	LEU	139	94.301	92.982	72.746	1.00	0.00	H
ATOM	1442	2HD1	LEU	139	94.379	94.064	75.041	1.00	0.00	H
ATOM	1443	3HD1	LEU	139	92.776	94.796	74.748	1.00	0.00	H
ATOM	1444	1HD1	LEU	139	92.958	93.031	74.876	1.00	0.00	H
ATOM	1445	2HD2	LEU	139	91.625	94.498	72.380	1.00	0.00	H
ATOM	1446	3HD2	LEU	139	92.420	93.425	71.210	1.00	0.00	H
ATOM	1447	1HD2	LEU	139	91.766	92.749	72.704	1.00	0.00	H
ATOM	1448	N	GLU	140	94.311	96.661	68.919	1.00	0.00	N
ATOM	1449	CA	GLU	140	95.583	97.311	68.479	1.00	0.00	C
ATOM	1450	C	GLU	140	96.622	96.377	67.752	1.00	0.00	C
ATOM	1451	O	GLU	140	96.907	95.279	68.222	1.00	0.00	O
ATOM	1452	CB	GLU	140	96.197	98.284	69.534	1.00	0.00	C
ATOM	1453	CG	GLU	140	96.556	99.716	69.056	1.00	0.00	C
ATOM	1454	CD	GLU	140	97.614	100.407	69.926	1.00	0.00	C
ATOM	1455	OE1	GLU	140	98.716	99.888	70.184	1.00	0.00	O
ATOM	1456	OE2	GLU	140	97.295	101.695	70.221	1.00	0.00	O
ATOM	1457	H	GLU	140	93.439	96.792	68.391	1.00	0.00	H
ATOM	1458	HA	GLU	140	95.204	97.973	67.674	1.00	0.00	H
ATOM	1459	1HB	GLU	140	95.535	98.373	70.417	1.00	0.00	H
ATOM	1460	2HB	GLU	140	97.116	97.812	69.926	1.00	0.00	H
ATOM	1461	1HG	GLU	140	96.948	99.703	68.025	1.00	0.00	H
ATOM	1462	2HG	GLU	140	95.644	100.338	69.008	1.00	0.00	H
ATOM	1463	N	LEU	141	97.189	96.813	66.605	1.00	0.00	N
ATOM	1464	CA	LEU	141	98.215	96.059	65.806	1.00	0.00	C
ATOM	1465	C	LEU	141	97.869	94.561	65.465	1.00	0.00	C
ATOM	1466	O	LEU	141	97.231	94.319	64.446	1.00	0.00	O
ATOM	1467	CB	LEU	141	99.684	96.288	66.287	1.00	0.00	C
ATOM	1468	CG	LEU	141	100.294	97.716	66.239	1.00	0.00	C
ATOM	1469	CD1	LEU	141	99.949	98.559	67.478	1.00	0.00	C
ATOM	1470	CD2	LEU	141	101.828	97.644	66.150	1.00	0.00	C
ATOM	1471	H	LEU	141	96.894	97.753	66.330	1.00	0.00	H
ATOM	1472	HA	LEU	141	98.193	96.531	64.805	1.00	0.00	H
ATOM	1473	1HB	LEU	141	99.800	95.860	67.293	1.00	0.00	H
ATOM	1474	2HB	LEU	141	100.316	95.635	65.650	1.00	0.00	H
ATOM	1475	HG	LEU	141	99.924	98.234	65.331	1.00	0.00	H
ATOM	1476	2HD1	LEU	141	98.865	98.650	67.627	1.00	0.00	H
ATOM	1477	3HD1	LEU	141	100.359	98.128	68.411	1.00	0.00	H
ATOM	1478	1HD1	LEU	141	100.344	99.590	67.401	1.00	0.00	H
ATOM	1479	2HD2	LEU	141	102.277	97.137	67.025	1.00	0.00	H
ATOM	1480	3HD2	LEU	141	102.157	97.089	65.253	1.00	0.00	H
ATOM	1481	1HD2	LEU	141	102.288	98.647	66.082	1.00	0.00	H
ATOM	1482	N	HIS	142	98.239	93.574	66.305	1.00	0.00	N
ATOM	1483	CA	HIS	142	97.890	92.130	66.120	1.00	0.00	C
ATOM	1484	C	HIS	142	96.376	91.786	65.867	1.00	0.00	C
ATOM	1485	O	HIS	142	96.077	91.082	64.902	1.00	0.00	O
ATOM	1486	CB	HIS	142	98.520	91.384	67.333	1.00	0.00	C
ATOM	1487	CG	HIS	142	98.401	89.863	67.314	1.00	0.00	C
ATOM	1488	ND1	HIS	142	99.032	89.064	66.378	1.00	0.00	N
ATOM	1489	CE1	HIS	142	98.517	87.850	66.743	1.00	0.00	C
ATOM	1490	NE2	HIS	142	97.673	87.762	67.818	1.00	0.00	N
ATOM	1491	CD2	HIS	142	97.591	89.095	68.166	1.00	0.00	C
ATOM	1492	H	HIS	142	98.568	93.935	67.207	1.00	0.00	H
ATOM	1493	HA	HIS	142	98.425	91.776	65.215	1.00	0.00	H
ATOM	1494	1HB	HIS	142	99.601	91.610	67.390	1.00	0.00	H
ATOM	1495	2HB	HIS	142	98.095	91.771	68.280	1.00	0.00	H
ATOM	1496	HE1	HIS	142	98.758	86.968	66.161	1.00	0.00	H
ATOM	1497	HE2	HIS	142	97.139	86.941	68.140	1.00	0.00	H
ATOM	1498	HD2	HIS	142	96.957	89.499	68.943	1.00	0.00	H
ATOM	1499	N	LYS	143	95.427	92.296	66.675	1.00	0.00	N
ATOM	1500	CA	LYS	143	93.966	92.168	66.366	1.00	0.00	C
ATOM	1501	C	LYS	143	93.456	92.911	65.071	1.00	0.00	C
ATOM	1502	O	LYS	143	92.547	92.416	64.401	1.00	0.00	O
ATOM	1503	CB	LYS	143	93.182	92.544	67.652	1.00	0.00	C
ATOM	1504	CG	LYS	143	91.694	92.119	67.639	1.00	0.00	C
ATOM	1505	CD	LYS	143	90.996	92.400	68.981	1.00	0.00	C
ATOM	1506	CE	LYS	143	89.522	91.976	68.981	1.00	0.00	C
ATOM	1507	NZ	LYS	143	88.936	92.262	70.305	1.00	0.00	N
ATOM	1508	1HZ	LYS	143	87.946	91.979	70.312	1.00	0.00	H
ATOM	1509	2HZ	LYS	143	89.448	91.737	71.029	1.00	0.00	H
ATOM	1510	3HZ	LYS	143	89.005	93.271	70.501	1.00	0.00	H

ATOM	1511	H	LYS	143	95.796	92.914	67.405	1.00	0.00	H
ATOM	1512	HA	LYS	143	93.768	91.094	66.174	1.00	0.00	H
ATOM	1513	1HB	LYS	143	93.663	92.071	68.532	1.00	0.00	H
ATOM	1514	2HB	LYS	143	93.260	93.634	67.831	1.00	0.00	H
ATOM	1515	1HG	LYS	143	91.157	92.643	66.822	1.00	0.00	H
ATOM	1516	2HG	LYS	143	91.612	91.041	67.399	1.00	0.00	H
ATOM	1517	1HD	LYS	143	91.533	91.864	69.788	1.00	0.00	H
ATOM	1518	2HD	LYS	143	91.083	93.480	69.220	1.00	0.00	H
ATOM	1519	1HE	LYS	143	88.963	92.511	68.187	1.00	0.00	H
ATOM	1520	2HE	LYS	143	89.428	90.895	68.753	1.00	0.00	H
ATOM	1521	N	ARG	144	94.052	94.055	64.693	0.00	0.00	N
ATOM	1522	CA	ARG	144	93.818	94.707	63.364	0.00	0.00	C
ATOM	1523	C	ARG	144	94.430	93.932	62.133	0.00	0.00	C
ATOM	1524	O	ARG	144	93.771	93.765	61.107	0.00	0.00	O
ATOM	1525	CB	ARG	144	94.325	96.187	63.398	0.00	0.00	C
ATOM	1526	CG	ARG	144	94.048	97.079	64.638	0.00	0.00	C
ATOM	1527	CD	ARG	144	92.575	97.236	65.036	0.00	0.00	C
ATOM	1528	NE	ARG	144	92.517	98.058	66.275	0.00	0.00	N
ATOM	1529	CZ	ARG	144	91.428	98.276	67.001	0.00	0.00	C
ATOM	1530	NH1	ARG	144	90.254	97.796	66.722	0.00	0.00	N
ATOM	1531	NH2	ARG	144	91.551	99.010	68.049	0.00	0.00	N
ATOM	1532	HE	ARG	144	93.394	98.494	66.595	1.00	0.00	H
ATOM	1533	H	ARG	144	94.877	94.270	65.261	0.00	0.00	H
ATOM	1534	HA	ARG	144	92.724	94.742	63.188	0.00	0.00	H
ATOM	1535	1HB	ARG	144	93.934	96.702	62.499	0.00	0.00	H
ATOM	1536	2HB	ARG	144	95.422	96.182	63.249	0.00	0.00	H
ATOM	1537	1HG	ARG	144	94.490	98.081	64.473	0.00	0.00	H
ATOM	1538	2HG	ARG	144	94.603	96.661	65.499	0.00	0.00	H
ATOM	1539	1HD	ARG	144	92.121	96.238	65.209	0.00	0.00	H
ATOM	1540	2HD	ARG	144	91.997	97.713	64.219	0.00	0.00	H
ATOM	1541	1HH1	ARG	144	89.492	98.028	67.359	0.00	0.00	H
ATOM	1542	2HH1	ARG	144	90.243	97.220	65.880	0.00	0.00	H
ATOM	1543	1HH2	ARG	144	90.714	99.175	68.606	0.00	0.00	H
ATOM	1544	2HH2	ARG	144	92.504	99.350	68.179	0.00	0.00	H
ATOM	1545	N	ARG	145	95.685	93.464	62.247	1.00	0.00	N
ATOM	1546	CA	ARG	145	96.370	92.597	61.243	1.00	0.00	C
ATOM	1547	C	ARG	145	95.872	91.111	61.094	1.00	0.00	C
ATOM	1548	O	ARG	145	96.228	90.473	60.101	1.00	0.00	O
ATOM	1549	CB	ARG	145	97.877	92.563	61.650	1.00	0.00	C
ATOM	1550	CG	ARG	145	98.679	93.889	61.575	1.00	0.00	C
ATOM	1551	CD	ARG	145	100.051	93.757	62.256	1.00	0.00	C
ATOM	1552	NE	ARG	145	100.752	95.066	62.215	1.00	0.00	N
ATOM	1553	CZ	ARG	145	102.002	95.278	62.604	1.00	0.00	C
ATOM	1554	NH1	ARG	145	102.785	94.365	63.098	1.00	0.00	N
ATOM	1555	NH2	ARG	145	102.465	96.470	62.475	1.00	0.00	N
ATOM	1556	HE	ARG	145	100.224	95.874	61.856	1.00	0.00	H
ATOM	1557	H	ARG	145	96.135	93.688	63.146	1.00	0.00	H
ATOM	1558	HA	ARG	145	96.281	93.057	60.240	1.00	0.00	H
ATOM	1559	1HB	ARG	145	97.951	92.141	62.674	1.00	0.00	H
ATOM	1560	2HB	ARG	145	98.410	91.821	61.021	1.00	0.00	H
ATOM	1561	1HG	ARG	145	98.805	94.204	60.520	1.00	0.00	H
ATOM	1562	2HG	ARG	145	98.115	94.711	62.056	1.00	0.00	H
ATOM	1563	1HD	ARG	145	99.923	93.427	63.309	1.00	0.00	H
ATOM	1564	2HD	ARG	145	100.648	92.971	61.751	1.00	0.00	H
ATOM	1565	2HH1	ARG	145	102.341	93.449	63.156	1.00	0.00	H
ATOM	1566	1HH1	ARG	145	103.735	94.640	63.347	1.00	0.00	H
ATOM	1567	1HH2	ARG	145	101.776	97.099	62.057	1.00	0.00	H
ATOM	1568	2HH2	ARG	145	103.434	96.635	62.741	1.00	0.00	H
ATOM	1569	N	LYS	146	95.154	90.529	62.082	1.00	0.00	N
ATOM	1570	CA	LYS	146	94.909	89.056	62.215	1.00	0.00	C
ATOM	1571	C	LYS	146	96.148	88.227	62.721	1.00	0.00	C
ATOM	1572	O	LYS	146	96.076	87.587	63.775	1.00	0.00	O
ATOM	1573	CB	LYS	146	94.152	88.452	60.992	1.00	0.00	C
ATOM	1574	CG	LYS	146	93.601	87.019	61.176	1.00	0.00	C
ATOM	1575	CD	LYS	146	92.958	86.485	59.881	1.00	0.00	C
ATOM	1576	CE	LYS	146	92.463	85.041	60.031	1.00	0.00	C
ATOM	1577	NZ	LYS	146	91.884	84.588	58.751	1.00	0.00	N
ATOM	1578	1HZ	LYS	146	91.550	83.618	58.848	1.00	0.00	H
ATOM	1579	2HZ	LYS	146	91.094	85.197	58.495	1.00	0.00	H
ATOM	1580	3HZ	LYS	146	92.603	84.630	58.014	1.00	0.00	H
ATOM	1581	H	LYS	146	95.036	91.156	62.887	1.00	0.00	H
ATOM	1582	HA	LYS	146	94.192	88.979	63.054	1.00	0.00	H
ATOM	1583	1HB	LYS	146	93.317	89.127	60.718	1.00	0.00	H

ATOM	1584	2HB	LYS	146	94.824	88.464	60.112	1.00	0.00	H
ATOM	1585	1HG	LYS	146	94.419	86.340	61.489	1.00	0.00	H
ATOM	1586	2HG	LYS	146	92.866	87.000	62.003	1.00	0.00	H
ATOM	1587	1HD	LYS	146	92.118	87.145	59.582	1.00	0.00	H
ATOM	1588	2HD	LYS	146	93.694	86.549	59.054	1.00	0.00	H
ATOM	1589	1HE	LYS	146	93.296	84.375	60.333	1.00	0.00	H
ATOM	1590	2HE	LYS	146	91.704	84.972	60.836	1.00	0.00	H
ATOM	1591	N	ALA	147	97.248	88.196	61.950	1.00	0.00	N
ATOM	1592	CA	ALA	147	98.402	87.294	62.187	1.00	0.00	C
ATOM	1593	C	ALA	147	99.779	87.983	61.895	1.00	0.00	C
ATOM	1594	O	ALA	147	99.933	88.722	60.915	1.00	0.00	O
ATOM	1595	CB	ALA	147	98.170	86.085	61.256	1.00	0.00	C
ATOM	1596	H	ALA	147	97.178	88.800	61.122	1.00	0.00	H
ATOM	1597	HA	ALA	147	98.408	86.934	63.237	1.00	0.00	H
ATOM	1598	2HB	ALA	147	97.255	85.528	61.536	1.00	0.00	H
ATOM	1599	3HB	ALA	147	98.071	86.380	60.195	1.00	0.00	H
ATOM	1600	1HB	ALA	147	99.006	85.368	61.308	1.00	0.00	H
ATOM	1601	N	LEU	148	100.806	87.700	62.716	1.00	0.00	N
ATOM	1602	CA	LEU	148	102.207	88.129	62.439	1.00	0.00	C
ATOM	1603	C	LEU	148	102.986	87.003	61.680	1.00	0.00	C
ATOM	1604	O	LEU	148	103.014	85.843	62.105	1.00	0.00	O
ATOM	1605	CB	LEU	148	102.939	88.519	63.757	1.00	0.00	C
ATOM	1606	CG	LEU	148	102.326	89.637	64.641	1.00	0.00	C
ATOM	1607	CD1	LEU	148	103.212	89.891	65.868	1.00	0.00	C
ATOM	1608	CD2	LEU	148	102.098	90.967	63.907	1.00	0.00	C
ATOM	1609	H	LEU	148	100.590	87.057	63.490	1.00	0.00	H
ATOM	1610	HA	LEU	148	102.200	89.037	61.803	1.00	0.00	H
ATOM	1611	1HB	LEU	148	103.042	87.607	64.378	1.00	0.00	H
ATOM	1612	2HB	LEU	148	103.981	88.795	63.509	1.00	0.00	H
ATOM	1613	HG	LEU	148	101.343	89.275	65.004	1.00	0.00	H
ATOM	1614	2HD1	LEU	148	103.436	88.954	66.407	1.00	0.00	H
ATOM	1615	3HD1	LEU	148	104.185	90.351	65.609	1.00	0.00	H
ATOM	1616	1HD1	LEU	148	102.720	90.564	66.595	1.00	0.00	H
ATOM	1617	2HD2	LEU	148	103.034	91.381	63.491	1.00	0.00	H
ATOM	1618	3HD2	LEU	148	101.382	90.848	63.072	1.00	0.00	H
ATOM	1619	1HD2	LEU	148	101.664	91.730	64.580	1.00	0.00	H
ATOM	1620	N	THR	149	103.648	87.338	60.563	1.00	0.00	N
ATOM	1621	CA	THR	149	104.435	86.350	59.754	1.00	0.00	C
ATOM	1622	C	THR	149	105.682	85.746	60.498	1.00	0.00	C
ATOM	1623	O	THR	149	106.190	86.324	61.461	1.00	0.00	O
ATOM	1624	CB	THR	149	104.837	86.961	58.370	1.00	0.00	C
ATOM	1625	OG1	THR	149	105.679	88.098	58.524	1.00	0.00	O
ATOM	1626	CG2	THR	149	103.673	87.383	57.459	1.00	0.00	C
ATOM	1627	H	THR	149	103.553	88.318	60.285	1.00	0.00	H
ATOM	1628	HA	THR	149	103.758	85.496	59.545	1.00	0.00	H
ATOM	1629	HB	THR	149	105.407	86.192	57.810	1.00	0.00	H
ATOM	1630	HG1	THR	149	105.422	88.711	57.831	1.00	0.00	H
ATOM	1631	1HG2	THR	149	104.024	87.738	56.472	1.00	0.00	H
ATOM	1632	2HG2	THR	149	102.982	86.539	57.266	1.00	0.00	H
ATOM	1633	3HG2	THR	149	103.065	88.194	57.904	1.00	0.00	H
ATOM	1634	N	GLU	150	106.193	84.586	60.038	0.00	0.00	N
ATOM	1635	CA	GLU	150	107.355	83.885	60.680	0.00	0.00	C
ATOM	1636	C	GLU	150	108.671	84.748	60.925	0.00	0.00	C
ATOM	1637	O	GLU	150	109.164	84.675	62.052	0.00	0.00	O
ATOM	1638	CB	GLU	150	107.587	82.517	59.960	0.00	0.00	C
ATOM	1639	CG	GLU	150	106.402	81.503	60.039	0.00	0.00	C
ATOM	1640	CD	GLU	150	106.509	80.210	59.224	0.00	0.00	C
ATOM	1641	OE1	GLU	150	107.099	79.207	59.610	0.00	0.00	O
ATOM	1642	OE2	GLU	150	105.835	80.283	58.040	0.00	0.00	O
ATOM	1643	H	GLU	150	105.612	84.128	59.330	0.00	0.00	H
ATOM	1644	HA	GLU	150	107.022	83.624	61.706	0.00	0.00	H
ATOM	1645	1HB	GLU	150	108.487	82.034	60.389	0.00	0.00	H
ATOM	1646	2HB	GLU	150	107.856	82.703	58.907	0.00	0.00	H
ATOM	1647	1HG	GLU	150	105.461	81.993	59.736	0.00	0.00	H
ATOM	1648	2HG	GLU	150	106.235	81.212	61.092	0.00	0.00	H
ATOM	1649	N	PRO	151	109.214	85.621	60.014	0.00	0.00	N
ATOM	1650	CA	PRO	151	110.199	86.694	60.384	0.00	0.00	C
ATOM	1651	CD	PRO	151	108.872	85.617	58.583	0.00	0.00	C
ATOM	1652	C	PRO	151	109.855	87.723	61.524	0.00	0.00	C
ATOM	1653	O	PRO	151	110.743	88.145	62.266	0.00	0.00	O
ATOM	1654	CB	PRO	151	110.413	87.422	59.037	0.00	0.00	C
ATOM	1655	CG	PRO	151	109.986	86.440	57.949	0.00	0.00	C
ATOM	1656	HA	PRO	151	111.150	86.203	60.668	0.00	0.00	H

ATOM	1657	1HD	PRO	151	107.885	86.088	58.412	0.00	0.00	H
ATOM	1658	2HD	PRO	151	108.856	84.598	58.157	0.00	0.00	H
ATOM	1659	1HB	PRO	151	111.462	87.754	58.917	0.00	0.00	H
ATOM	1660	2HB	PRO	151	109.787	88.335	58.968	0.00	0.00	H
ATOM	1661	1HG	PRO	151	110.834	85.785	57.690	0.00	0.00	H
ATOM	1662	2HG	PRO	151	109.669	86.944	57.018	0.00	0.00	H
ATOM	1663	N	GLU	152	108.587	88.146	61.648	1.00	0.00	N
ATOM	1664	CA	GLU	152	108.117	89.007	62.775	1.00	0.00	C
ATOM	1665	C	GLU	152	107.904	88.238	64.129	1.00	0.00	C
ATOM	1666	O	GLU	152	108.439	88.657	65.158	1.00	0.00	O
ATOM	1667	CB	GLU	152	106.855	89.756	62.250	1.00	0.00	C
ATOM	1668	CG	GLU	152	106.211	90.800	63.203	1.00	0.00	C
ATOM	1669	CD	GLU	152	106.987	92.086	63.492	1.00	0.00	C
ATOM	1670	OE1	GLU	152	108.200	92.220	63.370	1.00	0.00	O
ATOM	1671	OE2	GLU	152	106.172	93.078	63.939	1.00	0.00	O
ATOM	1672	H	GLU	152	107.932	87.605	61.072	1.00	0.00	H
ATOM	1673	HA	GLU	152	108.892	89.773	62.981	1.00	0.00	H
ATOM	1674	1HB	GLU	152	107.096	90.261	61.293	1.00	0.00	H
ATOM	1675	2HB	GLU	152	106.081	89.009	61.984	1.00	0.00	H
ATOM	1676	1HG	GLU	152	105.230	91.093	62.786	1.00	0.00	H
ATOM	1677	2HG	GLU	152	105.977	90.333	64.176	1.00	0.00	H
ATOM	1678	N	ALA	153	107.158	87.116	64.137	0.00	0.00	N
ATOM	1679	CA	ALA	153	107.037	86.226	65.325	0.00	0.00	C
ATOM	1680	C	ALA	153	108.359	85.596	65.902	0.00	0.00	C
ATOM	1681	O	ALA	153	108.492	85.516	67.125	0.00	0.00	O
ATOM	1682	CB	ALA	153	105.982	85.168	64.944	0.00	0.00	C
ATOM	1683	H	ALA	153	106.793	86.850	63.212	0.00	0.00	H
ATOM	1684	HA	ALA	153	106.608	86.829	66.151	0.00	0.00	H
ATOM	1685	1HB	ALA	153	105.751	84.502	65.795	0.00	0.00	H
ATOM	1686	2HB	ALA	153	105.021	85.624	64.636	0.00	0.00	H
ATOM	1687	3HB	ALA	153	106.317	84.525	64.108	0.00	0.00	H
ATOM	1688	N	ARG	154	109.343	85.199	65.066	0.00	0.00	N
ATOM	1689	CA	ARG	154	110.722	84.852	65.539	0.00	0.00	C
ATOM	1690	C	ARG	154	111.530	85.995	66.258	0.00	0.00	C
ATOM	1691	O	ARG	154	112.158	85.741	67.286	0.00	0.00	O
ATOM	1692	CB	ARG	154	111.503	84.146	64.390	0.00	0.00	C
ATOM	1693	CG	ARG	154	112.107	85.065	63.296	0.00	0.00	C
ATOM	1694	CD	ARG	154	113.543	85.528	63.593	0.00	0.00	C
ATOM	1695	NE	ARG	154	113.880	86.656	62.687	0.00	0.00	N
ATOM	1696	CZ	ARG	154	114.866	87.527	62.870	0.00	0.00	C
ATOM	1697	NH1	ARG	154	115.740	87.459	63.831	0.00	0.00	N
ATOM	1698	NH2	ARG	154	114.962	88.493	62.030	0.00	0.00	N
ATOM	1699	HE	ARG	154	113.299	86.772	61.844	1.00	0.00	H
ATOM	1700	H	ARG	154	109.127	85.334	64.069	0.00	0.00	H
ATOM	1701	HA	ARG	154	110.592	84.074	66.310	0.00	0.00	H
ATOM	1702	1HB	ARG	154	110.836	83.409	63.904	0.00	0.00	H
ATOM	1703	2HB	ARG	154	112.305	83.522	64.828	0.00	0.00	H
ATOM	1704	1HG	ARG	154	111.443	85.935	63.149	0.00	0.00	H
ATOM	1705	2HG	ARG	154	112.090	84.564	62.315	0.00	0.00	H
ATOM	1706	1HD	ARG	154	114.240	84.680	63.473	0.00	0.00	H
ATOM	1707	2HD	ARG	154	113.654	85.843	64.648	0.00	0.00	H
ATOM	1708	1HH1	ARG	154	116.480	88.160	63.838	0.00	0.00	H
ATOM	1709	2HH1	ARG	154	115.646	86.618	64.402	0.00	0.00	H
ATOM	1710	1HH2	ARG	154	115.697	89.181	62.187	0.00	0.00	H
ATOM	1711	2HH2	ARG	154	114.203	88.476	61.347	0.00	0.00	H
ATOM	1712	N	TYR	155	111.514	87.235	65.733	1.00	0.00	N
ATOM	1713	CA	TYR	155	112.066	88.440	66.422	1.00	0.00	C
ATOM	1714	C	TYR	155	111.457	88.734	67.843	1.00	0.00	C
ATOM	1715	O	TYR	155	112.186	89.051	68.784	1.00	0.00	O
ATOM	1716	CB	TYR	155	111.895	89.611	65.411	1.00	0.00	C
ATOM	1717	CG	TYR	155	112.698	90.878	65.739	1.00	0.00	C
ATOM	1718	CD1	TYR	155	113.979	91.045	65.204	1.00	0.00	C
ATOM	1719	CD2	TYR	155	112.161	91.879	66.559	1.00	0.00	C
ATOM	1720	CE1	TYR	155	114.708	92.198	65.479	1.00	0.00	C
ATOM	1721	CE2	TYR	155	112.900	93.027	66.840	1.00	0.00	C
ATOM	1722	CZ	TYR	155	114.171	93.185	66.296	1.00	0.00	C
ATOM	1723	OH	TYR	155	114.904	94.310	66.558	1.00	0.00	O
ATOM	1724	H	TYR	155	111.095	87.361	64.800	1.00	0.00	H
ATOM	1725	HA	TYR	155	113.152	88.277	66.573	1.00	0.00	H
ATOM	1726	1HB	TYR	155	112.182	89.280	64.391	1.00	0.00	H
ATOM	1727	2HB	TYR	155	110.823	89.866	65.305	1.00	0.00	H
ATOM	1728	HD1	TYR	155	114.411	90.280	64.573	1.00	0.00	H
ATOM	1729	HD2	TYR	155	111.176	91.762	66.990	1.00	0.00	H

ATOM	1730	HE1	TYR	155	115.698	92.323	65.073	1.00	0.00	H
ATOM	1731	HE2	TYR	155	112.486	93.787	67.484	1.00	0.00	H
ATOM	1732	HH	TYR	155	114.330	94.967	66.971	1.00	0.00	H
ATOM	1733	N	TYR	156	110.132	88.574	67.992	0.00	0.00	N
ATOM	1734	CA	TYR	156	109.433	88.599	69.304	0.00	0.00	C
ATOM	1735	C	TYR	156	109.852	87.428	70.275	0.00	0.00	C
ATOM	1736	O	TYR	156	110.195	87.710	71.422	0.00	0.00	O
ATOM	1737	CB	TYR	156	107.898	88.642	69.018	0.00	0.00	C
ATOM	1738	CG	TYR	156	107.223	89.943	68.497	0.00	0.00	C
ATOM	1739	CD1	TYR	156	107.798	90.774	67.520	0.00	0.00	C
ATOM	1740	CE1	TYR	156	107.141	91.923	67.090	0.00	0.00	C
ATOM	1741	CZ	TYR	156	105.895	92.247	67.606	0.00	0.00	C
ATOM	1742	OH	TYR	156	105.263	93.392	67.205	0.00	0.00	O
ATOM	1743	CE2	TYR	156	105.296	91.425	68.555	0.00	0.00	C
ATOM	1744	CD2	TYR	156	105.959	90.281	68.997	0.00	0.00	C
ATOM	1745	H	TYR	156	109.565	88.424	67.145	1.00	0.00	H
ATOM	1746	HA	TYR	156	109.702	89.539	69.829	0.00	0.00	H
ATOM	1747	1HB	TYR	156	107.396	88.358	69.964	0.00	0.00	H
ATOM	1748	2HB	TYR	156	107.629	87.819	68.330	0.00	0.00	H
ATOM	1749	HD1	TYR	156	108.758	90.552	67.084	0.00	0.00	H
ATOM	1750	HE1	TYR	156	107.610	92.568	66.361	0.00	0.00	H
ATOM	1751	HH	TYR	156	104.508	93.523	67.781	0.00	0.00	H
ATOM	1752	HE2	TYR	156	104.337	91.683	68.977	0.00	0.00	H
ATOM	1753	HD2	TYR	156	105.486	89.679	69.760	0.00	0.00	H
ATOM	1754	N	LEU	157	109.860	86.143	69.853	1.00	0.00	N
ATOM	1755	CA	LEU	157	110.345	85.012	70.711	1.00	0.00	C
ATOM	1756	C	LEU	157	111.873	84.971	71.073	1.00	0.00	C
ATOM	1757	O	LEU	157	112.208	84.574	72.191	1.00	0.00	O
ATOM	1758	CB	LEU	157	109.771	83.662	70.181	1.00	0.00	C
ATOM	1759	CG	LEU	157	110.541	82.934	69.039	1.00	0.00	C
ATOM	1760	CD1	LEU	157	111.558	81.907	69.572	1.00	0.00	C
ATOM	1761	CD2	LEU	157	109.575	82.206	68.098	1.00	0.00	C
ATOM	1762	H	LEU	157	109.582	86.019	68.870	1.00	0.00	H
ATOM	1763	HA	LEU	157	109.856	85.147	71.693	1.00	0.00	H
ATOM	1764	1HB	LEU	157	109.664	82.968	71.037	1.00	0.00	H
ATOM	1765	2HB	LEU	157	108.718	83.834	69.881	1.00	0.00	H
ATOM	1766	HG	LEU	157	111.088	83.689	68.443	1.00	0.00	H
ATOM	1767	2HD1	LEU	157	112.317	82.369	70.227	1.00	0.00	H
ATOM	1768	3HD1	LEU	157	111.074	81.105	70.159	1.00	0.00	H
ATOM	1769	1HD1	LEU	157	112.116	81.418	68.750	1.00	0.00	H
ATOM	1770	2HD2	LEU	157	108.993	81.441	68.635	1.00	0.00	H
ATOM	1771	3HD2	LEU	157	108.848	82.902	67.638	1.00	0.00	H
ATOM	1772	1HD2	LEU	157	110.101	81.700	67.267	1.00	0.00	H
ATOM	1773	N	ARG	158	112.794	85.339	70.162	1.00	0.00	N
ATOM	1774	CA	ARG	158	114.267	85.286	70.417	1.00	0.00	C
ATOM	1775	C	ARG	158	114.818	86.178	71.582	1.00	0.00	C
ATOM	1776	O	ARG	158	115.619	85.706	72.392	1.00	0.00	O
ATOM	1777	CB	ARG	158	115.007	85.449	69.057	1.00	0.00	C
ATOM	1778	CG	ARG	158	115.175	86.874	68.458	1.00	0.00	C
ATOM	1779	CD	ARG	158	116.540	87.524	68.779	1.00	0.00	C
ATOM	1780	NE	ARG	158	116.446	89.000	68.662	1.00	0.00	N
ATOM	1781	CZ	ARG	158	117.045	89.775	67.769	1.00	0.00	C
ATOM	1782	NH1	ARG	158	117.835	89.356	66.828	1.00	0.00	N
ATOM	1783	NH2	ARG	158	116.819	91.036	67.853	1.00	0.00	N
ATOM	1784	HE	ARG	158	115.849	89.477	69.353	1.00	0.00	H
ATOM	1785	H	ARG	158	112.401	85.649	69.259	1.00	0.00	H
ATOM	1786	HA	ARG	158	114.482	84.249	70.742	1.00	0.00	H
ATOM	1787	1HB	ARG	158	115.999	84.986	69.177	1.00	0.00	H
ATOM	1788	2HB	ARG	158	114.521	84.802	68.299	1.00	0.00	H
ATOM	1789	1HG	ARG	158	115.054	86.841	67.357	1.00	0.00	H
ATOM	1790	2HG	ARG	158	114.337	87.520	68.789	1.00	0.00	H
ATOM	1791	1HD	ARG	158	116.836	87.294	69.821	1.00	0.00	H
ATOM	1792	2HD	ARG	158	117.337	87.084	68.149	1.00	0.00	H
ATOM	1793	2HH1	ARG	158	117.958	88.343	66.791	1.00	0.00	H
ATOM	1794	1HH1	ARG	158	118.205	90.060	66.191	1.00	0.00	H
ATOM	1795	1HH2	ARG	158	116.085	91.238	68.536	1.00	0.00	H
ATOM	1796	2HH2	ARG	158	117.170	91.627	67.101	1.00	0.00	H
ATOM	1797	N	GLN	159	114.342	87.426	71.705	0.00	0.00	N
ATOM	1798	CA	GLN	159	114.561	88.275	72.911	0.00	0.00	C
ATOM	1799	C	GLN	159	113.899	87.764	74.246	0.00	0.00	C
ATOM	1800	O	GLN	159	114.458	87.994	75.318	0.00	0.00	O
ATOM	1801	CB	GLN	159	114.096	89.718	72.581	0.00	0.00	C
ATOM	1802	CG	GLN	159	114.776	90.433	71.381	0.00	0.00	C

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ATOM   1803  CD  GLN   159     114.427  91.912  71.236  0.00  0.00           C
ATOM   1804  OE1 GLN   159     113.474  92.320  70.582  0.00  0.00           O
ATOM   1805  NE2 GLN   159     115.171  92.782  71.861  0.00  0.00           N
ATOM   1806  H   GLN   159     113.734  87.719  70.929  0.00  0.00           H
ATOM   1807  HA  GLN   159     115.650  88.322  73.109  0.00  0.00           H
ATOM   1808 1HB  GLN   159     114.249  90.337  73.487  0.00  0.00           H
ATOM   1809 2HB  GLN   159     113.003  89.711  72.411  0.00  0.00           H
ATOM   1810 1HG  GLN   159     114.475  89.939  70.438  0.00  0.00           H
ATOM   1811 2HG  GLN   159     115.875  90.305  71.420  0.00  0.00           H
ATOM   1812 1HE2 GLN   159     115.731  92.400  72.632  0.00  0.00           H
ATOM   1813 2HE2 GLN   159     114.805  93.732  71.792  0.00  0.00           H
ATOM   1814  N   ILE   160     112.749  87.059  74.203  0.00  0.00           N
ATOM   1815  CA  ILE   160     112.178  86.320  75.382  0.00  0.00           C
ATOM   1816  C   ILE   160     113.065  85.090  75.820  0.00  0.00           C
ATOM   1817  O   ILE   160     113.349  84.959  77.011  0.00  0.00           O
ATOM   1818  CB  ILE   160     110.665  85.933  75.161  0.00  0.00           C
ATOM   1819  CG2 ILE   160     110.033  85.314  76.441  0.00  0.00           C
ATOM   1820  CG1 ILE   160     109.741  87.100  74.696  0.00  0.00           C
ATOM   1821  CD1 ILE   160     108.408  86.662  74.063  0.00  0.00           C
ATOM   1822  H   ILE   160     112.391  86.927  73.248  0.00  0.00           H
ATOM   1823  HA  ILE   160     112.195  87.020  76.242  0.00  0.00           H
ATOM   1824  HB  ILE   160     110.651  85.163  74.364  0.00  0.00           H
ATOM   1825 1HG2 ILE   160     108.989  84.988  76.278  0.00  0.00           H
ATOM   1826 2HG2 ILE   160     110.580  84.418  76.788  0.00  0.00           H
ATOM   1827 3HG2 ILE   160     110.020  86.029  77.284  0.00  0.00           H
ATOM   1828 1HG1 ILE   160     110.259  87.714  73.936  0.00  0.00           H
ATOM   1829 2HG1 ILE   160     109.554  87.808  75.526  0.00  0.00           H
ATOM   1830 1HD1 ILE   160     107.902  87.513  73.570  0.00  0.00           H
ATOM   1831 2HD1 ILE   160     108.545  85.892  73.285  0.00  0.00           H
ATOM   1832 3HD1 ILE   160     107.708  86.253  74.812  0.00  0.00           H
ATOM   1833  N   VAL   161     113.521  84.213  74.899  0.00  0.00           N
ATOM   1834  CA  VAL   161     114.529  83.137  75.205  0.00  0.00           C
ATOM   1835  C   VAL   161     115.907  83.685  75.750  0.00  0.00           C
ATOM   1836  O   VAL   161     116.400  83.167  76.752  0.00  0.00           O
ATOM   1837  CB  VAL   161     114.681  82.153  73.984  0.00  0.00           C
ATOM   1838  CG1 VAL   161     115.681  80.993  74.226  0.00  0.00           C
ATOM   1839  CG2 VAL   161     113.363  81.472  73.541  0.00  0.00           C
ATOM   1840  H   VAL   161     113.202  84.416  73.940  0.00  0.00           H
ATOM   1841  HA  VAL   161     114.115  82.533  76.037  0.00  0.00           H
ATOM   1842  HB  VAL   161     115.060  82.747  73.126  0.00  0.00           H
ATOM   1843 1HG1 VAL   161     115.804  80.350  73.333  0.00  0.00           H
ATOM   1844 2HG1 VAL   161     116.693  81.358  74.477  0.00  0.00           H
ATOM   1845 3HG1 VAL   161     115.368  80.335  75.059  0.00  0.00           H
ATOM   1846 1HG2 VAL   161     113.504  80.827  72.653  0.00  0.00           H
ATOM   1847 2HG2 VAL   161     112.928  80.840  74.338  0.00  0.00           H
ATOM   1848 3HG2 VAL   161     112.588  82.210  73.260  0.00  0.00           H
ATOM   1849  N   LEU   162     116.504  84.730  75.145  0.00  0.00           N
ATOM   1850  CA  LEU   162     117.649  85.484  75.753  0.00  0.00           C
ATOM   1851  C   LEU   162     117.378  86.204  77.127  0.00  0.00           C
ATOM   1852  O   LEU   162     118.260  86.217  77.988  0.00  0.00           O
ATOM   1853  CB  LEU   162     118.193  86.481  74.690  0.00  0.00           C
ATOM   1854  CG  LEU   162     118.906  85.886  73.448  0.00  0.00           C
ATOM   1855  CD1 LEU   162     119.135  86.980  72.393  0.00  0.00           C
ATOM   1856  CD2 LEU   162     120.255  85.243  73.811  0.00  0.00           C
ATOM   1857  H   LEU   162     116.028  85.052  74.289  0.00  0.00           H
ATOM   1858  HA  LEU   162     118.451  84.756  75.972  0.00  0.00           H
ATOM   1859 1HB  LEU   162     118.894  87.188  75.175  0.00  0.00           H
ATOM   1860 2HB  LEU   162     117.350  87.120  74.357  0.00  0.00           H
ATOM   1861  HG  LEU   162     118.252  85.114  72.991  0.00  0.00           H
ATOM   1862 1HD1 LEU   162     119.596  86.571  71.476  0.00  0.00           H
ATOM   1863 2HD1 LEU   162     118.185  87.454  72.080  0.00  0.00           H
ATOM   1864 3HD1 LEU   162     119.801  87.785  72.757  0.00  0.00           H
ATOM   1865 1HD2 LEU   162     120.769  84.844  72.918  0.00  0.00           H
ATOM   1866 2HD2 LEU   162     120.944  85.963  74.291  0.00  0.00           H
ATOM   1867 3HD2 LEU   162     120.136  84.390  74.502  0.00  0.00           H
ATOM   1868  N   GLY   163     116.183  86.782  77.352  1.00  0.00           N
ATOM   1869  CA  GLY   163     115.710  87.181  78.711  1.00  0.00           C
ATOM   1870  C   GLY   163     115.582  86.064  79.778  1.00  0.00           C
ATOM   1871  O   GLY   163     116.190  86.183  80.837  1.00  0.00           O
ATOM   1872  H   GLY   163     115.552  86.757  76.537  1.00  0.00           H
ATOM   1873 1HA  GLY   163     116.368  87.972  79.118  1.00  0.00           H
ATOM   1874 2HA  GLY   163     114.724  87.667  78.616  1.00  0.00           H
ATOM   1875  N   CYS   164     114.850  84.974  79.497  1.00  0.00           N
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ATOM	1876	CA	CYS	164	114.876	83.737	80.335	1.00	0.00	C
ATOM	1877	C	CYS	164	116.266	83.039	80.567	1.00	0.00	C
ATOM	1878	O	CYS	164	116.521	82.564	81.673	1.00	0.00	O
ATOM	1879	CB	CYS	164	113.829	82.778	79.729	1.00	0.00	C
ATOM	1880	SG	CYS	164	112.154	83.509	79.788	1.00	0.00	S
ATOM	1881	H	CYS	164	114.400	84.992	78.570	1.00	0.00	H
ATOM	1882	HA	CYS	164	114.518	84.010	81.346	1.00	0.00	H
ATOM	1883	1HB	CYS	164	114.081	82.520	78.681	1.00	0.00	H
ATOM	1884	2HB	CYS	164	113.813	81.822	80.285	1.00	0.00	H
ATOM	1885	HG	CYS	164	112.078	83.650	81.109	1.00	0.00	H
ATOM	1886	N	GLN	165	117.185	83.026	79.584	1.00	0.00	N
ATOM	1887	CA	GLN	165	118.630	82.717	79.812	1.00	0.00	C
ATOM	1888	C	GLN	165	119.377	83.597	80.884	1.00	0.00	C
ATOM	1889	O	GLN	165	120.137	83.048	81.686	1.00	0.00	O
ATOM	1890	CB	GLN	165	119.305	82.732	78.409	1.00	0.00	C
ATOM	1891	CG	GLN	165	120.812	82.361	78.337	1.00	0.00	C
ATOM	1892	CD	GLN	165	121.171	80.925	78.714	1.00	0.00	C
ATOM	1893	OE1	GLN	165	121.176	80.021	77.889	1.00	0.00	O
ATOM	1894	NE2	GLN	165	121.483	80.662	79.958	1.00	0.00	N
ATOM	1895	H	GLN	165	116.831	83.380	78.683	1.00	0.00	H
ATOM	1896	HA	GLN	165	118.685	81.679	80.192	1.00	0.00	H
ATOM	1897	1HB	GLN	165	118.748	82.064	77.721	1.00	0.00	H
ATOM	1898	2HB	GLN	165	119.186	83.742	77.971	1.00	0.00	H
ATOM	1899	1HG	GLN	165	121.163	82.514	77.300	1.00	0.00	H
ATOM	1900	2HG	GLN	165	121.416	83.072	78.933	1.00	0.00	H
ATOM	1901	1HE2	GLN	165	121.348	81.425	80.632	1.00	0.00	H
ATOM	1902	2HE2	GLN	165	121.686	79.679	80.146	1.00	0.00	H
ATOM	1903	N	TYR	166	119.158	84.923	80.915	0.00	0.00	N
ATOM	1904	CA	TYR	166	119.568	85.789	82.059	0.00	0.00	C
ATOM	1905	C	TYR	166	118.771	85.539	83.393	0.00	0.00	C
ATOM	1906	O	TYR	166	119.399	85.300	84.425	0.00	0.00	O
ATOM	1907	CB	TYR	166	119.502	87.256	81.545	0.00	0.00	C
ATOM	1908	CG	TYR	166	120.132	88.308	82.473	0.00	0.00	C
ATOM	1909	CD1	TYR	166	121.487	88.633	82.352	0.00	0.00	C
ATOM	1910	CE1	TYR	166	122.045	89.626	83.155	0.00	0.00	C
ATOM	1911	CZ	TYR	166	121.259	90.279	84.099	0.00	0.00	C
ATOM	1912	OH	TYR	166	121.795	91.289	84.845	0.00	0.00	O
ATOM	1913	CE2	TYR	166	119.916	89.950	84.239	0.00	0.00	C
ATOM	1914	CD2	TYR	166	119.349	88.973	83.422	0.00	0.00	C
ATOM	1915	H	TYR	166	118.685	85.361	80.112	1.00	0.00	H
ATOM	1916	HA	TYR	166	120.631	85.572	82.293	0.00	0.00	H
ATOM	1917	1HB	TYR	166	118.451	87.533	81.332	0.00	0.00	H
ATOM	1918	2HB	TYR	166	119.994	87.330	80.555	0.00	0.00	H
ATOM	1919	HD1	TYR	166	122.106	88.133	81.622	0.00	0.00	H
ATOM	1920	HE1	TYR	166	123.087	89.891	83.046	0.00	0.00	H
ATOM	1921	HH	TYR	166	122.244	91.892	84.240	0.00	0.00	H
ATOM	1922	HE2	TYR	166	119.310	90.457	84.974	0.00	0.00	H
ATOM	1923	HD2	TYR	166	118.302	88.727	83.543	0.00	0.00	H
ATOM	1924	N	LEU	167	117.424	85.573	83.383	0.00	0.00	N
ATOM	1925	CA	LEU	167	116.580	85.358	84.599	0.00	0.00	C
ATOM	1926	C	LEU	167	116.762	83.982	85.326	0.00	0.00	C
ATOM	1927	O	LEU	167	116.969	83.963	86.540	0.00	0.00	O
ATOM	1928	CB	LEU	167	115.083	85.622	84.256	0.00	0.00	C
ATOM	1929	CG	LEU	167	114.679	87.034	83.757	0.00	0.00	C
ATOM	1930	CD1	LEU	167	113.194	87.063	83.364	0.00	0.00	C
ATOM	1931	CD2	LEU	167	114.939	88.119	84.808	0.00	0.00	C
ATOM	1932	H	LEU	167	117.014	85.798	82.466	0.00	0.00	H
ATOM	1933	HA	LEU	167	116.884	86.113	85.350	0.00	0.00	H
ATOM	1934	1HB	LEU	167	114.473	85.389	85.151	0.00	0.00	H
ATOM	1935	2HB	LEU	167	114.764	84.870	83.510	0.00	0.00	H
ATOM	1936	HG	LEU	167	115.274	87.289	82.858	0.00	0.00	H
ATOM	1937	1HD1	LEU	167	112.894	88.053	82.971	0.00	0.00	H
ATOM	1938	2HD1	LEU	167	112.964	86.327	82.572	0.00	0.00	H
ATOM	1939	3HD1	LEU	167	112.532	86.847	84.222	0.00	0.00	H
ATOM	1940	1HD2	LEU	167	114.642	89.118	84.443	0.00	0.00	H
ATOM	1941	2HD2	LEU	167	114.388	87.929	85.748	0.00	0.00	H
ATOM	1942	3HD2	LEU	167	116.011	88.196	85.072	0.00	0.00	H
ATOM	1943	N	HIS	168	116.757	82.845	84.609	0.00	0.00	N
ATOM	1944	CA	HIS	168	117.105	81.512	85.190	0.00	0.00	C
ATOM	1945	C	HIS	168	118.576	81.396	85.749	0.00	0.00	C
ATOM	1946	O	HIS	168	118.773	80.818	86.819	0.00	0.00	O
ATOM	1947	CB	HIS	168	116.788	80.395	84.153	0.00	0.00	C
ATOM	1948	CG	HIS	168	115.353	80.235	83.617	0.00	0.00	C

ATOM	1949	ND1	HIS	168	114.199	80.809	84.143	0.00	0.00	N
ATOM	1950	CE1	HIS	168	113.278	80.323	83.255	0.00	0.00	C
ATOM	1951	NE2	HIS	168	113.675	79.497	82.239	0.00	0.00	N
ATOM	1952	CD2	HIS	168	115.034	79.451	82.498	0.00	0.00	C
ATOM	1953	H	HIS	168	116.578	82.972	83.603	0.00	0.00	H
ATOM	1954	HA	HIS	168	116.440	81.343	86.062	0.00	0.00	H
ATOM	1955	1HB	HIS	168	117.074	79.422	84.594	0.00	0.00	H
ATOM	1956	2HB	HIS	168	117.467	80.521	83.289	0.00	0.00	H
ATOM	1957	HE1	HIS	168	112.235	80.561	83.392	0.00	0.00	H
ATOM	1958	HE2	HIS	168	113.102	78.947	81.590	0.00	0.00	H
ATOM	1959	HD2	HIS	168	115.756	78.876	81.940	0.00	0.00	H
ATOM	1960	N	ARG	169	119.587	81.991	85.080	1.00	0.00	N
ATOM	1961	CA	ARG	169	120.937	82.244	85.682	1.00	0.00	C
ATOM	1962	C	ARG	169	120.977	83.160	86.968	1.00	0.00	C
ATOM	1963	O	ARG	169	121.743	82.871	87.888	1.00	0.00	O
ATOM	1964	CB	ARG	169	121.828	82.766	84.521	1.00	0.00	C
ATOM	1965	CG	ARG	169	123.343	82.852	84.825	1.00	0.00	C
ATOM	1966	CD	ARG	169	124.142	83.372	83.619	1.00	0.00	C
ATOM	1967	NE	ARG	169	125.581	83.393	83.981	1.00	0.00	N
ATOM	1968	CZ	ARG	169	126.573	83.759	83.183	1.00	0.00	C
ATOM	1969	NH1	ARG	169	126.421	84.150	81.954	1.00	0.00	N
ATOM	1970	NH2	ARG	169	127.763	83.721	83.667	1.00	0.00	N
ATOM	1971	HE	ARG	169	125.830	83.099	84.936	1.00	0.00	H
ATOM	1972	H	ARG	169	119.258	82.535	84.276	1.00	0.00	H
ATOM	1973	HA	ARG	169	121.348	81.266	86.002	1.00	0.00	H
ATOM	1974	1HB	ARG	169	121.700	82.114	83.635	1.00	0.00	H
ATOM	1975	2HB	ARG	169	121.462	83.761	84.197	1.00	0.00	H
ATOM	1976	1HG	ARG	169	123.525	83.511	85.698	1.00	0.00	H
ATOM	1977	2HG	ARG	169	123.729	81.859	85.131	1.00	0.00	H
ATOM	1978	1HD	ARG	169	123.973	82.723	82.737	1.00	0.00	H
ATOM	1979	2HD	ARG	169	123.797	84.390	83.344	1.00	0.00	H
ATOM	1980	2HH1	ARG	169	125.445	84.158	81.655	1.00	0.00	H
ATOM	1981	1HH1	ARG	169	127.263	84.410	81.442	1.00	0.00	H
ATOM	1982	1HH2	ARG	169	127.763	83.411	84.641	1.00	0.00	H
ATOM	1983	2HI2	ARG	169	128.535	84.007	83.067	1.00	0.00	H
ATOM	1984	N	ASN	170	120.138	84.208	87.078	1.00	0.00	N
ATOM	1985	CA	ASN	170	119.868	84.914	88.374	1.00	0.00	C
ATOM	1986	C	ASN	170	119.114	84.109	89.511	1.00	0.00	C
ATOM	1987	O	ASN	170	118.897	84.666	90.590	1.00	0.00	O
ATOM	1988	CB	ASN	170	119.043	86.208	88.075	1.00	0.00	C
ATOM	1989	CG	ASN	170	119.476	87.253	87.043	1.00	0.00	C
ATOM	1990	OD1	ASN	170	118.647	87.828	86.350	1.00	0.00	O
ATOM	1991	ND2	ASN	170	120.734	87.585	86.923	1.00	0.00	N
ATOM	1992	H	ASN	170	119.600	84.408	86.222	1.00	0.00	H
ATOM	1993	HA	ASN	170	120.836	85.216	88.819	1.00	0.00	H
ATOM	1994	1HB	ASN	170	118.016	85.911	87.792	1.00	0.00	H
ATOM	1995	2HB	ASN	170	118.903	86.769	89.016	1.00	0.00	H
ATOM	1996	1HD2	ASN	170	120.898	88.227	86.142	1.00	0.00	H
ATOM	1997	2HD2	ASN	170	121.406	86.966	87.382	1.00	0.00	H
ATOM	1998	N	ARG	171	118.659	82.858	89.280	1.00	0.00	N
ATOM	1999	CA	ARG	171	117.640	82.151	90.127	1.00	0.00	C
ATOM	2000	C	ARG	171	116.210	82.824	90.209	1.00	0.00	C
ATOM	2001	O	ARG	171	115.514	82.730	91.223	1.00	0.00	O
ATOM	2002	CB	ARG	171	118.236	81.706	91.497	1.00	0.00	C
ATOM	2003	CG	ARG	171	119.399	80.683	91.421	1.00	0.00	C
ATOM	2004	CD	ARG	171	119.917	80.277	92.807	1.00	0.00	C
ATOM	2005	NE	ARG	171	120.996	79.272	92.633	1.00	0.00	N
ATOM	2006	CZ	ARG	171	121.728	78.749	93.607	1.00	0.00	C
ATOM	2007	NH1	ARG	171	121.590	79.037	94.866	1.00	0.00	N
ATOM	2008	NH2	ARG	171	122.632	77.900	93.271	1.00	0.00	N
ATOM	2009	HE	ARG	171	121.194	78.955	91.674	1.00	0.00	H
ATOM	2010	H	ARG	171	118.968	82.485	88.374	1.00	0.00	H
ATOM	2011	HA	ARG	171	117.420	81.210	89.588	1.00	0.00	H
ATOM	2012	1HB	ARG	171	118.557	82.602	92.062	1.00	0.00	H
ATOM	2013	2HB	ARG	171	117.428	81.265	92.113	1.00	0.00	H
ATOM	2014	1HG	ARG	171	119.078	79.782	90.862	1.00	0.00	H
ATOM	2015	2HG	ARG	171	120.235	81.107	90.828	1.00	0.00	H
ATOM	2016	1HD	ARG	171	120.296	81.171	93.344	1.00	0.00	H
ATOM	2017	2HD	ARG	171	119.093	79.858	93.421	1.00	0.00	H
ATOM	2018	2HH1	ARG	171	120.858	79.727	95.037	1.00	0.00	H
ATOM	2019	1HH1	ARG	171	122.219	78.576	95.520	1.00	0.00	H
ATOM	2020	1HH2	ARG	171	122.663	77.768	92.258	1.00	0.00	H
ATOM	2021	2HH2	ARG	171	123.214	77.504	94.006	1.00	0.00	H

ATOM	2022	N	VAL	172	115.741	83.442	89.110	1.00	0.00	N
ATOM	2023	CA	VAL	172	114.438	84.169	89.046	1.00	0.00	C
ATOM	2024	C	VAL	172	113.496	83.370	88.083	1.00	0.00	C
ATOM	2025	O	VAL	172	113.552	83.505	86.855	1.00	0.00	O
ATOM	2026	CB	VAL	172	114.661	85.671	88.631	1.00	0.00	C
ATOM	2027	CG1	VAL	172	113.351	86.468	88.415	1.00	0.00	C
ATOM	2028	CG2	VAL	172	115.491	86.480	89.657	1.00	0.00	C
ATOM	2029	H	VAL	172	116.426	83.513	88.344	1.00	0.00	H
ATOM	2030	HA	VAL	172	113.959	84.202	90.047	1.00	0.00	H
ATOM	2031	HB	VAL	172	115.214	85.677	87.669	1.00	0.00	H
ATOM	2032	1HG1	VAL	172	112.732	86.513	89.332	1.00	0.00	H
ATOM	2033	2HG1	VAL	172	113.547	87.510	88.101	1.00	0.00	H
ATOM	2034	3HG1	VAL	172	112.721	86.025	87.621	1.00	0.00	H
ATOM	2035	2HG2	VAL	172	116.478	86.016	89.846	1.00	0.00	H
ATOM	2036	3HG2	VAL	172	115.697	87.510	89.309	1.00	0.00	H
ATOM	2037	1HG2	VAL	172	114.986	86.556	90.638	1.00	0.00	H
ATOM	2038	N	ILE	173	112.575	82.575	88.653	0.00	0.00	N
ATOM	2039	CA	ILE	173	111.447	81.954	87.886	0.00	0.00	C
ATOM	2040	C	ILE	173	110.383	83.074	87.611	0.00	0.00	C
ATOM	2041	O	ILE	173	109.709	83.512	88.544	0.00	0.00	O
ATOM	2042	CB	ILE	173	110.844	80.716	88.658	0.00	0.00	C
ATOM	2043	CG2	ILE	173	109.635	80.078	87.912	0.00	0.00	C
ATOM	2044	CG1	ILE	173	111.881	79.595	88.975	0.00	0.00	C
ATOM	2045	CD1	ILE	173	111.442	78.565	90.033	0.00	0.00	C
ATOM	2046	H	ILE	173	112.632	82.538	89.675	0.00	0.00	H
ATOM	2047	HA	ILE	173	111.836	81.577	86.918	0.00	0.00	H
ATOM	2048	HB	ILE	173	110.467	81.102	89.627	0.00	0.00	H
ATOM	2049	1HG2	ILE	173	109.151	79.289	88.517	0.00	0.00	H
ATOM	2050	2HG2	ILE	173	108.838	80.813	87.695	0.00	0.00	H
ATOM	2051	3HG2	ILE	173	109.929	79.606	86.958	0.00	0.00	H
ATOM	2052	1HG1	ILE	173	112.824	80.045	89.341	0.00	0.00	H
ATOM	2053	2HG1	ILE	173	112.172	79.077	88.044	0.00	0.00	H
ATOM	2054	1HD1	ILE	173	112.255	77.853	90.265	0.00	0.00	H
ATOM	2055	2HD1	ILE	173	111.160	79.050	90.988	0.00	0.00	H
ATOM	2056	3HD1	ILE	173	110.575	77.962	89.706	0.00	0.00	H
ATOM	2057	N	HIS	174	110.237	83.550	86.361	1.00	0.00	N
ATOM	2058	CA	HIS	174	109.317	84.693	86.059	1.00	0.00	C
ATOM	2059	C	HIS	174	107.793	84.449	86.376	1.00	0.00	C
ATOM	2060	O	HIS	174	107.197	85.215	87.138	1.00	0.00	O
ATOM	2061	CB	HIS	174	109.621	85.167	84.608	1.00	0.00	C
ATOM	2062	CG	HIS	174	108.991	86.510	84.245	1.00	0.00	C
ATOM	2063	ND1	HIS	174	109.547	87.720	84.610	1.00	0.00	N
ATOM	2064	CE1	HIS	174	108.528	88.561	84.240	1.00	0.00	C
ATOM	2065	NE2	HIS	174	107.408	88.047	83.646	1.00	0.00	N
ATOM	2066	CD2	HIS	174	107.722	86.700	83.677	1.00	0.00	C
ATOM	2067	H	HIS	174	111.089	83.401	85.808	1.00	0.00	H
ATOM	2068	HA	HIS	174	109.616	85.530	86.728	1.00	0.00	H
ATOM	2069	1HB	HIS	174	110.714	85.272	84.465	1.00	0.00	H
ATOM	2070	2HB	HIS	174	109.312	84.405	83.873	1.00	0.00	H
ATOM	2071	HE1	HIS	174	108.594	89.618	84.467	1.00	0.00	H
ATOM	2072	HE2	HIS	174	106.492	88.497	83.525	1.00	0.00	H
ATOM	2073	HD2	HIS	174	107.043	85.901	83.421	1.00	0.00	H
ATOM	2074	N	ARG	175	107.160	83.405	85.801	0.00	0.00	N
ATOM	2075	CA	ARG	175	105.738	83.015	86.076	0.00	0.00	C
ATOM	2076	C	ARG	175	104.626	83.935	85.455	0.00	0.00	C
ATOM	2077	O	ARG	175	103.710	83.427	84.802	0.00	0.00	O
ATOM	2078	CB	ARG	175	105.530	82.631	87.571	0.00	0.00	C
ATOM	2079	CG	ARG	175	104.378	81.637	87.838	0.00	0.00	C
ATOM	2080	CD	ARG	175	104.296	81.222	89.315	0.00	0.00	C
ATOM	2081	NE	ARG	175	103.290	80.140	89.415	0.00	0.00	N
ATOM	2082	CZ	ARG	175	102.838	79.593	90.531	0.00	0.00	C
ATOM	2083	NH1	ARG	175	103.214	79.931	91.729	0.00	0.00	N
ATOM	2084	NH2	ARG	175	101.966	78.668	90.400	0.00	0.00	N
ATOM	2085	HE	ARG	175	102.905	79.778	88.530	1.00	0.00	H
ATOM	2086	H	ARG	175	107.738	82.919	85.104	0.00	0.00	H
ATOM	2087	HA	ARG	175	105.622	82.068	85.513	0.00	0.00	H
ATOM	2088	1HB	ARG	175	105.397	83.551	88.171	0.00	0.00	H
ATOM	2089	2HB	ARG	175	106.465	82.177	87.958	0.00	0.00	H
ATOM	2090	1HG	ARG	175	104.517	80.733	87.210	0.00	0.00	H
ATOM	2091	2HG	ARG	175	103.406	82.064	87.515	0.00	0.00	H
ATOM	2092	1HD	ARG	175	104.009	82.089	89.943	0.00	0.00	H
ATOM	2093	2HD	ARG	175	105.280	80.863	89.681	0.00	0.00	H
ATOM	2094	1HH1	ARG	175	102.744	79.451	92.498	0.00	0.00	H

ATOM	2095	2HH1	ARG	175	103.889	80.695	91.751	0.00	0.00	H
ATOM	2096	1HH2	ARG	175	101.643	78.167	91.237	0.00	0.00	H
ATOM	2097	2HH2	ARG	175	101.804	78.446	89.417	0.00	0.00	H
ATOM	2098	N	ASP	176	104.702	85.268	85.615	0.00	0.00	N
ATOM	2099	CA	ASP	176	103.764	86.234	84.968	0.00	0.00	C
ATOM	2100	C	ASP	176	104.080	86.497	83.442	0.00	0.00	C
ATOM	2101	O	ASP	176	104.454	87.605	83.049	0.00	0.00	O
ATOM	2102	CB	ASP	176	103.818	87.483	85.894	0.00	0.00	C
ATOM	2103	CG	ASP	176	102.699	88.484	85.653	0.00	0.00	C
ATOM	2104	OD1	ASP	176	101.504	88.205	85.698	0.00	0.00	O
ATOM	2105	OD2	ASP	176	103.054	89.672	85.637	0.00	0.00	O
ATOM	2106	H	ASP	176	105.525	85.562	86.163	0.00	0.00	H
ATOM	2107	HA	ASP	176	102.735	85.823	85.015	0.00	0.00	H
ATOM	2108	1HB	ASP	176	104.797	87.993	85.798	0.00	0.00	H
ATOM	2109	2HB	ASP	176	103.748	87.209	86.962	0.00	0.00	H
ATOM	2110	N	LEU	177	103.924	85.481	82.572	0.00	0.00	N
ATOM	2111	CA	LEU	177	104.341	85.556	81.137	0.00	0.00	C
ATOM	2112	C	LEU	177	103.112	85.411	80.177	0.00	0.00	C
ATOM	2113	O	LEU	177	102.648	84.308	79.872	0.00	0.00	O
ATOM	2114	CB	LEU	177	105.476	84.511	80.915	0.00	0.00	C
ATOM	2115	CG	LEU	177	106.235	84.562	79.560	0.00	0.00	C
ATOM	2116	CD1	LEU	177	106.906	85.921	79.284	0.00	0.00	C
ATOM	2117	CD2	LEU	177	107.333	83.485	79.529	0.00	0.00	C
ATOM	2118	H	LEU	177	103.702	84.587	83.030	0.00	0.00	H
ATOM	2119	HA	LEU	177	104.805	86.542	80.937	0.00	0.00	H
ATOM	2120	1HB	LEU	177	105.054	83.496	81.051	0.00	0.00	H
ATOM	2121	2HB	LEU	177	106.224	84.609	81.725	0.00	0.00	H
ATOM	2122	HG	LEU	177	105.517	84.348	78.741	0.00	0.00	H
ATOM	2123	1HD1	LEU	177	107.505	85.902	78.353	0.00	0.00	H
ATOM	2124	2HD1	LEU	177	106.167	86.732	79.150	0.00	0.00	H
ATOM	2125	3HD1	LEU	177	107.586	86.228	80.101	0.00	0.00	H
ATOM	2126	1HD2	LEU	177	107.855	83.463	78.556	0.00	0.00	H
ATOM	2127	2HD2	LEU	177	108.102	83.646	80.307	0.00	0.00	H
ATOM	2128	3HD2	LEU	177	106.926	82.471	79.685	0.00	0.00	H
ATOM	2129	N	LYS	178	102.583	86.554	79.709	0.00	0.00	N
ATOM	2130	CA	LYS	178	101.463	86.610	78.722	0.00	0.00	C
ATOM	2131	C	LYS	178	101.689	87.771	77.676	0.00	0.00	C
ATOM	2132	O	LYS	178	102.744	88.413	77.632	0.00	0.00	O
ATOM	2133	CB	LYS	178	100.114	86.647	79.527	0.00	0.00	C
ATOM	2134	CG	LYS	178	99.771	88.005	80.244	0.00	0.00	C
ATOM	2135	CD	LYS	178	98.457	88.773	79.928	0.00	0.00	C
ATOM	2136	CE	LYS	178	98.363	90.078	80.774	0.00	0.00	C
ATOM	2137	NZ	LYS	178	97.371	91.082	80.284	0.00	0.00	N
ATOM	2138	1HZ	LYS	178	96.334	90.864	80.118	1.00	0.00	H
ATOM	2139	2HZ	LYS	178	97.357	92.061	80.681	1.00	0.00	H
ATOM	2140	3HZ	LYS	178	97.360	91.463	79.301	1.00	0.00	H
ATOM	2141	H	LYS	178	103.132	87.388	79.934	0.00	0.00	H
ATOM	2142	HA	LYS	178	101.469	85.678	78.119	0.00	0.00	H
ATOM	2143	1HB	LYS	178	100.182	85.941	80.379	0.00	0.00	H
ATOM	2144	2HB	LYS	178	99.318	86.209	78.895	0.00	0.00	H
ATOM	2145	1HG	LYS	178	100.614	88.710	80.085	0.00	0.00	H
ATOM	2146	2HG	LYS	178	99.828	87.850	81.343	0.00	0.00	H
ATOM	2147	1HD	LYS	178	97.563	88.150	80.119	0.00	0.00	H
ATOM	2148	2HD	LYS	178	98.407	89.015	78.850	0.00	0.00	H
ATOM	2149	1HE	LYS	178	99.353	90.577	80.849	0.00	0.00	H
ATOM	2150	2HE	LYS	178	98.140	89.833	81.834	0.00	0.00	H
ATOM	2151	N	LEU	179	100.665	88.092	76.867	1.00	0.00	N
ATOM	2152	CA	LEU	179	100.661	89.288	75.979	1.00	0.00	C
ATOM	2153	C	LEU	179	100.758	90.666	76.713	1.00	0.00	C
ATOM	2154	O	LEU	179	101.659	91.433	76.379	1.00	0.00	O
ATOM	2155	CB	LEU	179	99.451	89.228	75.007	1.00	0.00	C
ATOM	2156	CG	LEU	179	99.463	88.132	73.904	1.00	0.00	C
ATOM	2157	CD1	LEU	179	98.968	86.763	74.404	1.00	0.00	C
ATOM	2158	CD2	LEU	179	98.584	88.550	72.712	1.00	0.00	C
ATOM	2159	H	LEU	179	99.878	87.438	76.888	1.00	0.00	H
ATOM	2160	HA	LEU	179	101.577	89.250	75.358	1.00	0.00	H
ATOM	2161	1HB	LEU	179	98.498	89.208	75.572	1.00	0.00	H
ATOM	2162	2HB	LEU	179	99.425	90.204	74.488	1.00	0.00	H
ATOM	2163	HG	LEU	179	100.496	88.021	73.518	1.00	0.00	H
ATOM	2164	2HD1	LEU	179	99.607	86.339	75.196	1.00	0.00	H
ATOM	2165	3HD1	LEU	179	97.932	86.801	74.789	1.00	0.00	H
ATOM	2166	1HD1	LEU	179	98.988	86.014	73.593	1.00	0.00	H
ATOM	2167	2HD2	LEU	179	97.524	88.698	72.994	1.00	0.00	H

ATOM	2168	3HD2	LEU	179	98.936	89.497	72.259	1.00	0.00	H
ATOM	2169	1HD2	LEU	179	98.605	87.800	71.899	1.00	0.00	H
ATOM	2170	N	GLY	180	99.916	90.992	77.712	1.00	0.00	N
ATOM	2171	CA	GLY	180	100.099	92.232	78.527	1.00	0.00	C
ATOM	2172	C	GLY	180	101.529	92.588	79.036	1.00	0.00	C
ATOM	2173	O	GLY	180	102.069	93.647	78.710	1.00	0.00	O
ATOM	2174	H	GLY	180	99.039	90.461	77.744	1.00	0.00	H
ATOM	2175	1HA	GLY	180	99.812	93.071	77.875	1.00	0.00	H
ATOM	2176	2HA	GLY	180	99.394	92.319	79.367	1.00	0.00	H
ATOM	2177	N	ASN	181	102.174	91.645	79.727	0.00	0.00	N
ATOM	2178	CA	ASN	181	103.474	91.871	80.434	0.00	0.00	C
ATOM	2179	C	ASN	181	104.829	91.922	79.623	0.00	0.00	C
ATOM	2180	O	ASN	181	105.920	91.917	80.207	0.00	0.00	O
ATOM	2181	CB	ASN	181	103.567	90.754	81.519	0.00	0.00	C
ATOM	2182	CG	ASN	181	102.405	90.641	82.505	0.00	0.00	C
ATOM	2183	OD1	ASN	181	101.450	89.904	82.283	0.00	0.00	O
ATOM	2184	ND2	ASN	181	102.429	91.382	83.570	0.00	0.00	N
ATOM	2185	H	ASN	181	101.561	90.881	80.025	0.00	0.00	H
ATOM	2186	HA	ASN	181	103.420	92.840	80.969	0.00	0.00	H
ATOM	2187	1HB	ASN	181	104.500	90.872	82.106	0.00	0.00	H
ATOM	2188	2HB	ASN	181	103.685	89.766	81.039	0.00	0.00	H
ATOM	2189	1HD2	ASN	181	102.021	90.827	84.338	0.00	0.00	H
ATOM	2190	2HD2	ASN	181	103.337	91.837	83.699	0.00	0.00	H
ATOM	2191	N	LEU	182	104.794	92.001	78.289	0.00	0.00	N
ATOM	2192	CA	LEU	182	106.015	92.163	77.449	0.00	0.00	C
ATOM	2193	C	LEU	182	105.850	93.462	76.595	0.00	0.00	C
ATOM	2194	O	LEU	182	104.848	93.643	75.902	0.00	0.00	O
ATOM	2195	CB	LEU	182	106.188	90.902	76.560	0.00	0.00	C
ATOM	2196	CG	LEU	182	106.477	89.531	77.242	0.00	0.00	C
ATOM	2197	CD1	LEU	182	106.212	88.418	76.223	0.00	0.00	C
ATOM	2198	CD2	LEU	182	107.914	89.431	77.773	0.00	0.00	C
ATOM	2199	H	LEU	182	103.841	92.184	77.945	0.00	0.00	H
ATOM	2200	HA	LEU	182	106.927	92.272	78.072	0.00	0.00	H
ATOM	2201	1HB	LEU	182	106.998	91.117	75.844	0.00	0.00	H
ATOM	2202	2HB	LEU	182	105.275	90.809	75.941	0.00	0.00	H
ATOM	2203	HG	LEU	182	105.775	89.389	78.091	0.00	0.00	H
ATOM	2204	1HD1	LEU	182	106.449	87.416	76.624	0.00	0.00	H
ATOM	2205	2HD1	LEU	182	105.148	88.392	75.917	0.00	0.00	H
ATOM	2206	3HD1	LEU	182	106.808	88.561	75.304	0.00	0.00	H
ATOM	2207	1HD2	LEU	182	108.125	88.438	78.211	0.00	0.00	H
ATOM	2208	2HD2	LEU	182	108.666	89.603	76.980	0.00	0.00	H
ATOM	2209	3HD2	LEU	182	108.102	90.172	78.570	0.00	0.00	H
ATOM	2210	N	PHE	183	106.816	94.384	76.619	1.00	0.00	N
ATOM	2211	CA	PHE	183	106.566	95.801	76.213	1.00	0.00	C
ATOM	2212	C	PHE	183	107.378	96.162	74.934	1.00	0.00	C
ATOM	2213	O	PHE	183	108.602	96.004	74.910	1.00	0.00	O
ATOM	2214	CB	PHE	183	106.879	96.721	77.437	1.00	0.00	C
ATOM	2215	CG	PHE	183	105.873	96.583	78.598	1.00	0.00	C
ATOM	2216	CD1	PHE	183	104.710	97.353	78.601	1.00	0.00	C
ATOM	2217	CE1	PHE	183	103.664	97.046	79.467	1.00	0.00	C
ATOM	2218	CZ	PHE	183	103.797	96.002	80.375	1.00	0.00	C
ATOM	2219	CE2	PHE	183	104.987	95.288	80.441	1.00	0.00	C
ATOM	2220	CD2	PHE	183	106.024	95.575	79.557	1.00	0.00	C
ATOM	2221	H	PHE	183	107.542	94.195	77.325	1.00	0.00	H
ATOM	2222	HA	PHE	183	105.494	95.964	75.974	1.00	0.00	H
ATOM	2223	1HB	PHE	183	107.909	96.554	77.805	1.00	0.00	H
ATOM	2224	2HB	PHE	183	106.890	97.776	77.103	1.00	0.00	H
ATOM	2225	HD1	PHE	183	104.614	98.187	77.924	1.00	0.00	H
ATOM	2226	HE1	PHE	183	102.761	97.638	79.466	1.00	0.00	H
ATOM	2227	HZ	PHE	183	102.988	95.770	81.054	1.00	0.00	H
ATOM	2228	HE2	PHE	183	105.094	94.496	81.163	1.00	0.00	H
ATOM	2229	HD2	PHE	183	106.917	94.968	79.579	1.00	0.00	H
ATOM	2230	N	LEU	184	106.730	96.690	73.873	1.00	0.00	N
ATOM	2231	CA	LEU	184	107.416	97.309	72.691	1.00	0.00	C
ATOM	2232	C	LEU	184	108.064	98.692	73.028	1.00	0.00	C
ATOM	2233	O	LEU	184	107.333	99.660	73.283	1.00	0.00	O
ATOM	2234	CB	LEU	184	106.409	97.532	71.512	1.00	0.00	C
ATOM	2235	CG	LEU	184	106.138	96.389	70.506	1.00	0.00	C
ATOM	2236	CD1	LEU	184	105.052	96.846	69.514	1.00	0.00	C
ATOM	2237	CD2	LEU	184	107.372	96.012	69.667	1.00	0.00	C
ATOM	2238	H	LEU	184	105.739	96.918	74.050	1.00	0.00	H
ATOM	2239	HA	LEU	184	108.217	96.630	72.340	1.00	0.00	H
ATOM	2240	1HB	LEU	184	105.456	97.912	71.919	1.00	0.00	H

ATOM	2241	2HB	LEU	184	106.746	98.394	70.898	1.00	0.00	H
ATOM	2242	HG	LEU	184	105.777	95.497	71.059	1.00	0.00	H
ATOM	2243	2HD1	LEU	184	104.139	97.190	70.031	1.00	0.00	H
ATOM	2244	3HD1	LEU	184	105.390	97.690	68.883	1.00	0.00	H
ATOM	2245	1HD1	LEU	184	104.757	96.030	68.831	1.00	0.00	H
ATOM	2246	2HD2	LEU	184	107.705	96.837	69.013	1.00	0.00	H
ATOM	2247	3HD2	LEU	184	108.239	95.724	70.287	1.00	0.00	H
ATOM	2248	1HD2	LEU	184	107.163	95.145	69.011	1.00	0.00	H
ATOM	2249	N	ASN	185	109.403	98.774	73.058	1.00	0.00	N
ATOM	2250	CA	ASN	185	110.106	100.086	73.132	1.00	0.00	C
ATOM	2251	C	ASN	185	110.042	100.930	71.806	1.00	0.00	C
ATOM	2252	O	ASN	185	109.564	100.485	70.758	1.00	0.00	O
ATOM	2253	CB	ASN	185	111.522	99.846	73.732	1.00	0.00	C
ATOM	2254	CG	ASN	185	112.608	99.236	72.837	1.00	0.00	C
ATOM	2255	OD1	ASN	185	112.593	99.298	71.615	1.00	0.00	O
ATOM	2256	ND2	ASN	185	113.632	98.680	73.422	1.00	0.00	N
ATOM	2257	H	ASN	185	109.889	97.875	72.930	1.00	0.00	H
ATOM	2258	HA	ASN	185	109.576	100.716	73.879	1.00	0.00	H
ATOM	2259	1HB	ASN	185	111.919	100.816	74.083	1.00	0.00	H
ATOM	2260	2HB	ASN	185	111.419	99.249	74.657	1.00	0.00	H
ATOM	2261	1HD2	ASN	185	114.326	98.305	72.770	1.00	0.00	H
ATOM	2262	2HD2	ASN	185	113.566	98.525	74.431	1.00	0.00	H
ATOM	2263	N	GLU	186	110.562	102.162	71.853	1.00	0.00	N
ATOM	2264	CA	GLU	186	110.544	103.106	70.696	1.00	0.00	C
ATOM	2265	C	GLU	186	111.399	102.718	69.427	1.00	0.00	C
ATOM	2266	O	GLU	186	111.099	103.204	68.337	1.00	0.00	O
ATOM	2267	CB	GLU	186	110.887	104.518	71.262	1.00	0.00	C
ATOM	2268	CG	GLU	186	109.836	105.203	72.195	1.00	0.00	C
ATOM	2269	CD	GLU	186	109.642	104.655	73.619	1.00	0.00	C
ATOM	2270	OE1	GLU	186	110.476	103.990	74.228	1.00	0.00	O
ATOM	2271	OE2	GLU	186	108.515	104.880	74.100	1.00	0.00	O
ATOM	2272	H	GLU	186	110.799	102.491	72.797	1.00	0.00	H
ATOM	2273	HA	GLU	186	109.504	103.157	70.315	1.00	0.00	H
ATOM	2274	1HB	GLU	186	111.880	104.501	71.757	1.00	0.00	H
ATOM	2275	2HB	GLU	186	111.034	105.199	70.400	1.00	0.00	H
ATOM	2276	1HG	GLU	186	110.104	106.268	72.311	1.00	0.00	H
ATOM	2277	2HG	GLU	186	108.852	105.215	71.690	1.00	0.00	H
ATOM	2278	N	ASP	187	112.403	101.825	69.536	1.00	0.00	N
ATOM	2279	CA	ASP	187	112.999	101.111	68.358	1.00	0.00	C
ATOM	2280	C	ASP	187	112.360	99.707	67.989	1.00	0.00	C
ATOM	2281	O	ASP	187	112.928	98.972	67.175	1.00	0.00	O
ATOM	2282	CB	ASP	187	114.526	100.991	68.633	1.00	0.00	C
ATOM	2283	CG	ASP	187	115.313	102.299	68.593	1.00	0.00	C
ATOM	2284	OD1	ASP	187	115.655	102.860	67.559	1.00	0.00	O
ATOM	2285	OD2	ASP	187	115.596	102.774	69.835	1.00	0.00	O
ATOM	2286	H	ASP	187	112.486	101.438	70.483	1.00	0.00	H
ATOM	2287	HA	ASP	187	112.875	101.719	67.437	1.00	0.00	H
ATOM	2288	1HB	ASP	187	114.712	100.468	69.590	1.00	0.00	H
ATOM	2289	2HB	ASP	187	114.992	100.341	67.870	1.00	0.00	H
ATOM	2290	N	LEU	188	111.182	99.345	68.536	1.00	0.00	N
ATOM	2291	CA	LEU	188	110.435	98.074	68.258	1.00	0.00	C
ATOM	2292	C	LEU	188	111.031	96.740	68.850	1.00	0.00	C
ATOM	2293	O	LEU	188	110.984	95.685	68.210	1.00	0.00	O
ATOM	2294	CB	LEU	188	109.963	97.964	66.770	1.00	0.00	C
ATOM	2295	CG	LEU	188	109.099	99.113	66.185	1.00	0.00	C
ATOM	2296	CD1	LEU	188	108.906	98.904	64.675	1.00	0.00	C
ATOM	2297	CD2	LEU	188	107.720	99.221	66.860	1.00	0.00	C
ATOM	2298	H	LEU	188	110.807	100.045	69.191	1.00	0.00	H
ATOM	2299	HA	LEU	188	109.504	98.180	68.844	1.00	0.00	H
ATOM	2300	1HB	LEU	188	110.866	97.831	66.144	1.00	0.00	H
ATOM	2301	2HB	LEU	188	109.408	97.014	66.643	1.00	0.00	H
ATOM	2302	HG	LEU	188	109.638	100.073	66.327	1.00	0.00	H
ATOM	2303	2HD1	LEU	188	109.876	98.865	64.143	1.00	0.00	H
ATOM	2304	3HD1	LEU	188	108.372	97.962	64.446	1.00	0.00	H
ATOM	2305	1HD1	LEU	188	108.330	99.729	64.216	1.00	0.00	H
ATOM	2306	2HD2	LEU	188	107.141	98.282	66.782	1.00	0.00	H
ATOM	2307	3HD2	LEU	188	107.809	99.465	67.935	1.00	0.00	H
ATOM	2308	1HD2	LEU	188	107.108	100.025	66.411	1.00	0.00	H
ATOM	2309	N	GLU	189	111.538	96.755	70.097	1.00	0.00	N
ATOM	2310	CA	GLU	189	112.173	95.567	70.749	1.00	0.00	C
ATOM	2311	C	GLU	189	111.436	95.126	72.067	1.00	0.00	C
ATOM	2312	O	GLU	189	110.715	95.897	72.708	1.00	0.00	O
ATOM	2313	CB	GLU	189	113.678	95.893	71.008	1.00	0.00	C

ATOM	2314	CG	GLU	189	114.656	95.681	69.821	1.00	0.00	C
ATOM	2315	CD	GLU	189	114.692	96.837	68.832	1.00	0.00	C
ATOM	2316	OE1	GLU	189	115.281	97.892	69.046	1.00	0.00	O
ATOM	2317	OE2	GLU	189	113.970	96.585	67.707	1.00	0.00	O
ATOM	2318	H	GLU	189	111.640	97.704	70.480	1.00	0.00	H
ATOM	2319	HA	GLU	189	112.131	94.686	70.075	1.00	0.00	H
ATOM	2320	1HB	GLU	189	113.790	96.916	71.405	1.00	0.00	H
ATOM	2321	2HB	GLU	189	114.042	95.267	71.843	1.00	0.00	H
ATOM	2322	1HG	GLU	189	115.685	95.563	70.206	1.00	0.00	H
ATOM	2323	2HG	GLU	189	114.440	94.731	69.294	1.00	0.00	H
ATOM	2324	N	VAL	190	111.664	93.866	72.489	1.00	0.00	N
ATOM	2325	CA	VAL	190	111.100	93.293	73.754	1.00	0.00	C
ATOM	2326	C	VAL	190	111.790	93.877	75.036	1.00	0.00	C
ATOM	2327	O	VAL	190	112.974	93.637	75.298	1.00	0.00	O
ATOM	2328	CB	VAL	190	111.177	91.721	73.750	1.00	0.00	C
ATOM	2329	CG1	VAL	190	110.578	91.047	75.010	1.00	0.00	C
ATOM	2330	CG2	VAL	190	110.495	91.026	72.548	1.00	0.00	C
ATOM	2331	H	VAL	190	112.242	93.298	71.855	1.00	0.00	H
ATOM	2332	HA	VAL	190	110.025	93.542	73.801	1.00	0.00	H
ATOM	2333	HB	VAL	190	112.252	91.463	73.722	1.00	0.00	H
ATOM	2334	1HG1	VAL	190	109.496	91.252	75.118	1.00	0.00	H
ATOM	2335	2HG1	VAL	190	110.706	89.949	74.991	1.00	0.00	H
ATOM	2336	3HG1	VAL	190	111.068	91.390	75.941	1.00	0.00	H
ATOM	2337	2HG2	VAL	190	110.881	91.382	71.576	1.00	0.00	H
ATOM	2338	3HG2	VAL	190	110.658	89.933	72.556	1.00	0.00	H
ATOM	2339	1HG2	VAL	190	109.401	91.178	72.544	1.00	0.00	H
ATOM	2340	N	LYS	191	110.996	94.554	75.872	1.00	0.00	N
ATOM	2341	CA	LYS	191	111.369	94.885	77.269	1.00	0.00	C
ATOM	2342	C	LYS	191	110.423	94.113	78.258	1.00	0.00	C
ATOM	2343	O	LYS	191	109.215	94.364	78.306	1.00	0.00	O
ATOM	2344	CB	LYS	191	111.259	96.423	77.448	1.00	0.00	C
ATOM	2345	CG	LYS	191	112.257	97.343	76.706	1.00	0.00	C
ATOM	2346	CD	LYS	191	113.703	97.231	77.229	1.00	0.00	C
ATOM	2347	CE	LYS	191	114.545	98.495	76.998	1.00	0.00	C
ATOM	2348	NZ	LYS	191	115.860	98.307	77.636	1.00	0.00	N
ATOM	2349	1HZ	LYS	191	116.437	99.148	77.489	1.00	0.00	H
ATOM	2350	2HZ	LYS	191	115.733	98.151	78.646	1.00	0.00	H
ATOM	2351	3HZ	LYS	191	116.331	97.491	77.220	1.00	0.00	H
ATOM	2352	H	LYS	191	110.119	94.893	75.451	1.00	0.00	H
ATOM	2353	HA	LYS	191	112.417	94.601	77.489	1.00	0.00	H
ATOM	2354	1HB	LYS	191	110.229	96.745	77.190	1.00	0.00	H
ATOM	2355	2HB	LYS	191	111.347	96.649	78.525	1.00	0.00	H
ATOM	2356	1HG	LYS	191	112.222	97.146	75.616	1.00	0.00	H
ATOM	2357	2HG	LYS	191	111.899	98.383	76.832	1.00	0.00	H
ATOM	2358	1HD	LYS	191	113.684	97.025	78.314	1.00	0.00	H
ATOM	2359	2HD	LYS	191	114.192	96.343	76.780	1.00	0.00	H
ATOM	2360	1HE	LYS	191	114.675	98.701	75.921	1.00	0.00	H
ATOM	2361	2HE	LYS	191	114.048	99.385	77.436	1.00	0.00	H
ATOM	2362	N	ILE	192	110.954	93.189	79.078	1.00	0.00	N
ATOM	2363	CA	ILE	192	110.156	92.448	80.114	1.00	0.00	C
ATOM	2364	C	ILE	192	109.807	93.417	81.306	1.00	0.00	C
ATOM	2365	O	ILE	192	110.706	93.999	81.924	1.00	0.00	O
ATOM	2366	CB	ILE	192	110.905	91.140	80.577	1.00	0.00	C
ATOM	2367	CG1	ILE	192	111.266	90.151	79.424	1.00	0.00	C
ATOM	2368	CG2	ILE	192	110.090	90.351	81.640	1.00	0.00	C
ATOM	2369	CD1	ILE	192	112.362	89.124	79.760	1.00	0.00	C
ATOM	2370	H	ILE	192	111.953	92.986	78.923	1.00	0.00	H
ATOM	2371	HA	ILE	192	109.209	92.115	79.643	1.00	0.00	H
ATOM	2372	HB	ILE	192	111.853	91.469	81.050	1.00	0.00	H
ATOM	2373	1HG1	ILE	192	110.364	89.623	79.069	1.00	0.00	H
ATOM	2374	2HG1	ILE	192	111.620	90.711	78.536	1.00	0.00	H
ATOM	2375	2HG2	ILE	192	109.842	90.969	82.524	1.00	0.00	H
ATOM	2376	3HG2	ILE	192	109.133	89.964	81.241	1.00	0.00	H
ATOM	2377	1HG2	ILE	192	110.648	89.485	82.042	1.00	0.00	H
ATOM	2378	2HD1	ILE	192	113.309	89.619	80.049	1.00	0.00	H
ATOM	2379	3HD1	ILE	192	112.073	88.451	80.588	1.00	0.00	H
ATOM	2380	1HD1	ILE	192	112.580	88.482	78.887	1.00	0.00	H
ATOM	2381	N	GLY	193	108.501	93.593	81.560	1.00	0.00	N
ATOM	2382	CA	GLY	193	107.981	94.465	82.644	1.00	0.00	C
ATOM	2383	C	GLY	193	106.797	93.807	83.394	1.00	0.00	C
ATOM	2384	O	GLY	193	106.069	92.963	82.867	1.00	0.00	O
ATOM	2385	H	GLY	193	107.857	92.935	81.093	1.00	0.00	H
ATOM	2386	1HA	GLY	193	108.780	94.742	83.361	1.00	0.00	H

ATOM	2387	2HA	GLY	193	107.620	95.417	82.214	1.00	0.00	H
ATOM	2388	N	ASP	194	106.620	94.204	84.651	0.00	0.00	N
ATOM	2389	CA	ASP	194	105.779	93.470	85.637	0.00	0.00	C
ATOM	2390	C	ASP	194	106.338	92.050	86.040	0.00	0.00	C
ATOM	2391	O	ASP	194	106.282	91.059	85.311	0.00	0.00	O
ATOM	2392	CB	ASP	194	104.243	93.694	85.490	0.00	0.00	C
ATOM	2393	CG	ASP	194	103.710	94.969	86.165	0.00	0.00	C
ATOM	2394	OD1	ASP	194	102.591	94.994	86.709	0.00	0.00	O
ATOM	2395	OD2	ASP	194	104.420	95.994	86.207	0.00	0.00	O
ATOM	2396	H	ASP	194	107.243	94.956	84.952	0.00	0.00	H
ATOM	2397	HA	ASP	194	106.000	94.081	86.538	0.00	0.00	H
ATOM	2398	1HB	ASP	194	103.702	92.835	85.929	0.00	0.00	H
ATOM	2399	2HB	ASP	194	103.950	93.706	84.427	0.00	0.00	H
ATOM	2400	N	PHE	195	106.971	92.028	87.220	0.00	0.00	N
ATOM	2401	CA	PHE	195	107.659	90.844	87.809	0.00	0.00	C
ATOM	2402	C	PHE	195	106.955	90.346	89.118	0.00	0.00	C
ATOM	2403	O	PHE	195	107.603	89.677	89.928	0.00	0.00	O
ATOM	2404	CB	PHE	195	109.123	91.329	88.053	0.00	0.00	C
ATOM	2405	CG	PHE	195	110.056	91.346	86.828	0.00	0.00	C
ATOM	2406	CD1	PHE	195	110.856	90.237	86.538	0.00	0.00	C
ATOM	2407	CE1	PHE	195	111.733	90.267	85.457	0.00	0.00	C
ATOM	2408	CZ	PHE	195	111.821	91.406	84.661	0.00	0.00	C
ATOM	2409	CE2	PHE	195	111.028	92.514	84.943	0.00	0.00	C
ATOM	2410	CD2	PHE	195	110.140	92.480	86.015	0.00	0.00	C
ATOM	2411	H	PHE	195	106.824	92.881	87.779	0.00	0.00	H
ATOM	2412	HA	PHE	195	107.709	89.937	87.162	0.00	0.00	H
ATOM	2413	1HB	PHE	195	109.585	90.688	88.817	0.00	0.00	H
ATOM	2414	2HB	PHE	195	109.136	92.321	88.548	0.00	0.00	H
ATOM	2415	HD1	PHE	195	110.792	89.343	87.141	0.00	0.00	H
ATOM	2416	HE1	PHE	195	112.334	89.398	85.231	0.00	0.00	H
ATOM	2417	HZ	PHE	195	112.500	91.427	83.821	0.00	0.00	H
ATOM	2418	HE2	PHE	195	111.092	93.402	84.334	0.00	0.00	H
ATOM	2419	HD2	PHE	195	109.522	93.343	86.222	0.00	0.00	H
ATOM	2420	N	GLY	196	105.650	90.587	89.364	0.00	0.00	N
ATOM	2421	CA	GLY	196	105.014	90.327	90.689	0.00	0.00	C
ATOM	2422	C	GLY	196	104.105	89.088	90.820	0.00	0.00	C
ATOM	2423	O	GLY	196	102.957	89.227	91.239	0.00	0.00	O
ATOM	2424	H	GLY	196	105.226	91.180	88.638	0.00	0.00	H
ATOM	2425	1HA	GLY	196	104.419	91.219	90.959	0.00	0.00	H
ATOM	2426	2HA	GLY	196	105.762	90.262	91.504	0.00	0.00	H
ATOM	2427	N	LEU	197	104.634	87.889	90.543	1.00	0.00	N
ATOM	2428	CA	LEU	197	104.022	86.603	91.006	1.00	0.00	C
ATOM	2429	C	LEU	197	105.151	85.715	91.663	1.00	0.00	C
ATOM	2430	O	LEU	197	105.867	86.202	92.541	1.00	0.00	O
ATOM	2431	CB	LEU	197	103.184	85.943	89.856	1.00	0.00	C
ATOM	2432	CG	LEU	197	101.879	86.642	89.386	1.00	0.00	C
ATOM	2433	CD1	LEU	197	101.258	85.871	88.209	1.00	0.00	C
ATOM	2434	CD2	LEU	197	100.819	86.751	90.496	1.00	0.00	C
ATOM	2435	H	LEU	197	105.635	87.961	90.323	1.00	0.00	H
ATOM	2436	HA	LEU	197	103.337	86.799	91.855	1.00	0.00	H
ATOM	2437	1HB	LEU	197	103.851	85.796	88.985	1.00	0.00	H
ATOM	2438	2HB	LEU	197	102.903	84.921	90.170	1.00	0.00	H
ATOM	2439	HG	LEU	197	102.132	87.665	89.038	1.00	0.00	H
ATOM	2440	2HD1	LEU	197	101.973	85.727	87.381	1.00	0.00	H
ATOM	2441	3HD1	LEU	197	100.903	84.864	88.502	1.00	0.00	H
ATOM	2442	1HD1	LEU	197	100.391	86.412	87.783	1.00	0.00	H
ATOM	2443	2HD2	LEU	197	100.543	85.768	90.917	1.00	0.00	H
ATOM	2444	3HD2	LEU	197	101.167	87.379	91.337	1.00	0.00	H
ATOM	2445	1HD2	LEU	197	99.890	87.224	90.127	1.00	0.00	H
ATOM	2446	N	ALA	198	105.281	84.402	91.365	0.00	0.00	N
ATOM	2447	CA	ALA	198	106.339	83.495	91.934	0.00	0.00	C
ATOM	2448	C	ALA	198	106.806	83.637	93.440	0.00	0.00	C
ATOM	2449	O	ALA	198	108.002	83.748	93.727	0.00	0.00	O
ATOM	2450	CB	ALA	198	107.503	83.535	90.916	0.00	0.00	C
ATOM	2451	H	ALA	198	104.748	84.147	90.531	0.00	0.00	H
ATOM	2452	HA	ALA	198	105.931	82.469	91.885	0.00	0.00	H
ATOM	2453	1HB	ALA	198	108.291	82.802	91.167	0.00	0.00	H
ATOM	2454	2HB	ALA	198	107.191	83.322	89.879	0.00	0.00	H
ATOM	2455	3HB	ALA	198	107.996	84.527	90.905	0.00	0.00	H
ATOM	2456	N	THR	199	105.868	83.616	94.406	0.00	0.00	N
ATOM	2457	CA	THR	199	106.156	84.018	95.827	0.00	0.00	C
ATOM	2458	C	THR	199	106.899	82.955	96.723	0.00	0.00	C
ATOM	2459	O	THR	199	106.343	82.424	97.690	0.00	0.00	O

ATOM	2460	CB	THR	199	104.846	84.607	96.453	0.00	0.00	C
ATOM	2461	OG1	THR	199	105.108	85.041	97.781	0.00	0.00	O
ATOM	2462	CG2	THR	199	103.621	83.679	96.562	0.00	0.00	C
ATOM	2463	H	THR	199	104.928	83.743	94.023	0.00	0.00	H
ATOM	2464	HA	THR	199	106.844	84.891	95.797	0.00	0.00	H
ATOM	2465	HB	THR	199	104.555	85.498	95.858	0.00	0.00	H
ATOM	2466	HG1	THR	199	105.389	84.253	98.258	0.00	0.00	H
ATOM	2467	1HG2	THR	199	103.274	83.329	95.574	0.00	0.00	H
ATOM	2468	2HG2	THR	199	103.828	82.784	97.176	0.00	0.00	H
ATOM	2469	3HG2	THR	199	102.768	84.204	97.033	0.00	0.00	H
ATOM	2470	N	LYS	200	108.191	82.708	96.444	0.00	0.00	N
ATOM	2471	CA	LYS	200	109.045	81.751	97.211	0.00	0.00	C
ATOM	2472	C	LYS	200	110.269	82.493	97.854	0.00	0.00	C
ATOM	2473	O	LYS	200	110.965	83.267	97.191	0.00	0.00	O
ATOM	2474	CB	LYS	200	109.511	80.590	96.281	0.00	0.00	C
ATOM	2475	CG	LYS	200	108.392	79.733	95.634	0.00	0.00	C
ATOM	2476	CD	LYS	200	108.929	78.488	94.901	0.00	0.00	C
ATOM	2477	CE	LYS	200	107.840	77.788	94.074	0.00	0.00	C
ATOM	2478	NZ	LYS	200	108.399	76.594	93.408	0.00	0.00	N
ATOM	2479	1HZ	LYS	200	107.662	76.132	92.856	1.00	0.00	H
ATOM	2480	2HZ	LYS	200	109.168	76.877	92.784	1.00	0.00	H
ATOM	2481	3HZ	LYS	200	108.757	75.940	94.118	1.00	0.00	H
ATOM	2482	H	LYS	200	108.518	83.167	95.581	0.00	0.00	H
ATOM	2483	HA	LYS	200	108.457	81.285	98.030	0.00	0.00	H
ATOM	2484	1HB	LYS	200	110.160	81.001	95.481	0.00	0.00	H
ATOM	2485	2HB	LYS	200	110.174	79.924	96.865	0.00	0.00	H
ATOM	2486	1HG	LYS	200	107.653	79.425	96.400	0.00	0.00	H
ATOM	2487	2HG	LYS	200	107.826	80.368	94.923	0.00	0.00	H
ATOM	2488	1HD	LYS	200	109.766	78.777	94.234	0.00	0.00	H
ATOM	2489	2HD	LYS	200	109.366	77.785	95.637	0.00	0.00	H
ATOM	2490	1HE	LYS	200	106.978	77.501	94.711	0.00	0.00	H
ATOM	2491	2HE	LYS	200	107.440	78.483	93.308	0.00	0.00	H
ATOM	2492	N	VAL	201	110.533	82.262	99.151	0.00	0.00	N
ATOM	2493	CA	VAL	201	111.582	83.002	99.926	0.00	0.00	C
ATOM	2494	C	VAL	201	112.931	82.205	100.056	0.00	0.00	C
ATOM	2495	O	VAL	201	112.932	80.973	100.172	0.00	0.00	O
ATOM	2496	CB	VAL	201	110.952	83.444	101.300	0.00	0.00	C
ATOM	2497	CG1	VAL	201	110.769	82.319	102.349	0.00	0.00	C
ATOM	2498	CG2	VAL	201	111.719	84.604	101.969	0.00	0.00	C
ATOM	2499	H	VAL	201	109.948	81.547	99.591	0.00	0.00	H
ATOM	2500	HA	VAL	201	111.822	83.938	99.379	0.00	0.00	H
ATOM	2501	HB	VAL	201	109.942	83.850	101.080	0.00	0.00	H
ATOM	2502	1HG1	VAL	201	111.738	81.929	102.713	0.00	0.00	H
ATOM	2503	2HG1	VAL	201	110.206	82.666	103.235	0.00	0.00	H
ATOM	2504	3HG1	VAL	201	110.214	81.455	101.938	0.00	0.00	H
ATOM	2505	1HG2	VAL	201	112.741	84.312	102.280	0.00	0.00	H
ATOM	2506	2HG2	VAL	201	111.820	85.473	101.292	0.00	0.00	H
ATOM	2507	3HG2	VAL	201	111.200	84.973	102.874	0.00	0.00	H
ATOM	2508	N	GLU	202	114.083	82.901	100.125	0.00	0.00	N
ATOM	2509	CA	GLU	202	115.425	82.250	100.286	0.00	0.00	C
ATOM	2510	C	GLU	202	115.779	81.725	101.739	0.00	0.00	C
ATOM	2511	O	GLU	202	116.881	81.934	102.253	0.00	0.00	O
ATOM	2512	CB	GLU	202	116.504	83.217	99.708	0.00	0.00	C
ATOM	2513	CG	GLU	202	116.458	83.535	98.184	0.00	0.00	C
ATOM	2514	CD	GLU	202	115.676	84.788	97.775	0.00	0.00	C
ATOM	2515	OE1	GLU	202	114.539	85.053	98.156	0.00	0.00	O
ATOM	2516	OE2	GLU	202	116.386	85.585	96.932	0.00	0.00	O
ATOM	2517	H	GLU	202	114.001	83.871	99.795	0.00	0.00	H
ATOM	2518	HA	GLU	202	115.455	81.342	99.651	0.00	0.00	H
ATOM	2519	1HB	GLU	202	116.534	84.153	100.302	0.00	0.00	H
ATOM	2520	2HB	GLU	202	117.493	82.758	99.902	0.00	0.00	H
ATOM	2521	1HG	GLU	202	117.496	83.646	97.815	0.00	0.00	H
ATOM	2522	2HG	GLU	202	116.054	82.676	97.616	0.00	0.00	H
ATOM	2523	N	TYR	203	114.863	80.962	102.354	0.00	0.00	N
ATOM	2524	CA	TYR	203	115.139	80.119	103.556	0.00	0.00	C
ATOM	2525	C	TYR	203	114.495	78.695	103.433	0.00	0.00	C
ATOM	2526	O	TYR	203	115.206	77.708	103.643	0.00	0.00	O
ATOM	2527	CB	TYR	203	114.729	80.840	104.875	0.00	0.00	C
ATOM	2528	CG	TYR	203	115.716	81.901	105.398	0.00	0.00	C
ATOM	2529	CD1	TYR	203	116.989	81.520	105.840	0.00	0.00	C
ATOM	2530	CE1	TYR	203	117.875	82.471	106.344	0.00	0.00	C
ATOM	2531	CZ	TYR	203	117.489	83.805	106.423	0.00	0.00	C
ATOM	2532	OH	TYR	203	118.352	84.738	106.929	0.00	0.00	O

ATOM	2533	CE2	TYR	203	116.225	84.194	105.991	0.00	0.00	C
ATOM	2534	CD2	TYR	203	115.340	83.246	105.477	0.00	0.00	C
ATOM	2535	H	TYR	203	113.907	80.956	101.972	1.00	0.00	H
ATOM	2536	HA	TYR	203	116.228	79.912	103.608	0.00	0.00	H
ATOM	2537	1HB	TYR	203	113.711	81.261	104.769	0.00	0.00	H
ATOM	2538	2HB	TYR	203	114.617	80.092	105.682	0.00	0.00	H
ATOM	2539	HD1	TYR	203	117.300	80.485	105.787	0.00	0.00	H
ATOM	2540	HE1	TYR	203	118.858	82.164	106.672	0.00	0.00	H
ATOM	2541	HH	TYR	203	119.183	84.305	107.133	0.00	0.00	H
ATOM	2542	HE2	TYR	203	115.933	85.231	106.059	0.00	0.00	H
ATOM	2543	HD2	TYR	203	114.361	83.561	105.145	0.00	0.00	H
ATOM	2544	N	ASP	204	113.189	78.546	103.110	0.00	0.00	N
ATOM	2545	CA	ASP	204	112.574	77.215	102.817	0.00	0.00	C
ATOM	2546	C	ASP	204	111.617	77.238	101.564	0.00	0.00	C
ATOM	2547	O	ASP	204	110.886	78.205	101.331	0.00	0.00	O
ATOM	2548	CB	ASP	204	111.973	76.596	104.114	0.00	0.00	C
ATOM	2549	CG	ASP	204	110.524	76.932	104.462	0.00	0.00	C
ATOM	2550	OD1	ASP	204	110.164	77.963	105.017	0.00	0.00	O
ATOM	2551	OD2	ASP	204	109.676	75.937	104.080	0.00	0.00	O
ATOM	2552	H	ASP	204	112.693	79.423	102.920	0.00	0.00	H
ATOM	2553	HA	ASP	204	113.401	76.532	102.528	0.00	0.00	H
ATOM	2554	1HB	ASP	204	112.050	75.497	104.043	0.00	0.00	H
ATOM	2555	2HB	ASP	204	112.599	76.844	104.991	0.00	0.00	H
ATOM	2556	N	GLY	205	111.602	76.142	100.783	0.00	0.00	N
ATOM	2557	CA	GLY	205	110.724	76.006	99.584	0.00	0.00	C
ATOM	2558	C	GLY	205	109.511	75.068	99.784	0.00	0.00	C
ATOM	2559	O	GLY	205	109.682	73.872	100.024	0.00	0.00	O
ATOM	2560	H	GLY	205	112.181	75.370	101.128	0.00	0.00	H
ATOM	2561	1HA	GLY	205	110.407	76.994	99.196	0.00	0.00	H
ATOM	2562	2HA	GLY	205	111.323	75.579	98.760	0.00	0.00	H
ATOM	2563	N	GLU	206	108.290	75.605	99.660	0.00	0.00	N
ATOM	2564	CA	GLU	206	107.034	74.858	99.972	0.00	0.00	C
ATOM	2565	C	GLU	206	105.858	75.267	99.020	0.00	0.00	C
ATOM	2566	O	GLU	206	105.527	76.451	98.906	0.00	0.00	O
ATOM	2567	CB	GLU	206	106.695	75.043	101.487	0.00	0.00	C
ATOM	2568	CG	GLU	206	106.381	76.487	101.985	0.00	0.00	C
ATOM	2569	CD	GLU	206	106.297	76.676	103.499	0.00	0.00	C
ATOM	2570	OE1	GLU	206	107.039	76.129	104.309	0.00	0.00	O
ATOM	2571	OE2	GLU	206	105.335	77.567	103.853	0.00	0.00	O
ATOM	2572	H	GLU	206	108.289	76.621	99.527	0.00	0.00	H
ATOM	2573	HA	GLU	206	107.213	73.774	99.821	0.00	0.00	H
ATOM	2574	1HB	GLU	206	105.848	74.381	101.750	0.00	0.00	H
ATOM	2575	2HB	GLU	206	107.545	74.637	102.075	0.00	0.00	H
ATOM	2576	1HG	GLU	206	107.156	77.189	101.629	0.00	0.00	H
ATOM	2577	2HG	GLU	206	105.439	76.843	101.526	0.00	0.00	H
ATOM	2578	N	ARG	207	105.178	74.299	98.371	0.00	0.00	N
ATOM	2579	CA	ARG	207	103.984	74.593	97.511	0.00	0.00	C
ATOM	2580	C	ARG	207	102.644	74.622	98.338	0.00	0.00	C
ATOM	2581	O	ARG	207	101.731	73.817	98.148	0.00	0.00	O
ATOM	2582	CB	ARG	207	103.948	73.615	96.295	0.00	0.00	C
ATOM	2583	CG	ARG	207	105.115	73.695	95.268	0.00	0.00	C
ATOM	2584	CD	ARG	207	106.268	72.718	95.557	0.00	0.00	C
ATOM	2585	NE	ARG	207	107.373	72.962	94.591	0.00	0.00	N
ATOM	2586	CZ	ARG	207	108.655	73.134	94.889	0.00	0.00	C
ATOM	2587	NH1	ARG	207	109.140	73.144	96.096	0.00	0.00	N
ATOM	2588	NH2	ARG	207	109.474	73.306	93.911	0.00	0.00	N
ATOM	2589	HE	ARG	207	107.118	73.002	93.594	1.00	0.00	H
ATOM	2590	H	ARG	207	105.521	73.344	98.513	0.00	0.00	H
ATOM	2591	HA	ARG	207	104.084	75.603	97.065	0.00	0.00	H
ATOM	2592	1HB	ARG	207	103.801	72.574	96.640	0.00	0.00	H
ATOM	2593	2HB	ARG	207	103.016	73.828	95.733	0.00	0.00	H
ATOM	2594	1HG	ARG	207	104.731	73.468	94.252	0.00	0.00	H
ATOM	2595	2HG	ARG	207	105.498	74.731	95.192	0.00	0.00	H
ATOM	2596	1HD	ARG	207	106.593	72.797	96.609	0.00	0.00	H
ATOM	2597	2HD	ARG	207	105.910	71.676	95.436	0.00	0.00	H
ATOM	2598	1HH1	ARG	207	110.147	73.271	96.191	0.00	0.00	H
ATOM	2599	2HH1	ARG	207	108.436	73.002	96.820	0.00	0.00	H
ATOM	2600	1HH2	ARG	207	109.015	73.300	92.994	0.00	0.00	H
ATOM	2601	2HH2	ARG	207	110.458	73.437	94.135	0.00	0.00	H
ATOM	2602	N	LYS	208	102.551	75.594	99.257	0.00	0.00	N
ATOM	2603	CA	LYS	208	101.367	75.800	100.154	0.00	0.00	C
ATOM	2604	C	LYS	208	100.318	76.879	99.671	0.00	0.00	C
ATOM	2605	O	LYS	208	99.196	76.904	100.180	0.00	0.00	O

ATOM	2606	CB	LYS	208	102.023	76.067	101.541	0.00	0.00	C
ATOM	2607	CG	LYS	208	101.078	76.180	102.758	0.00	0.00	C
ATOM	2608	CD	LYS	208	101.870	76.109	104.081	0.00	0.00	C
ATOM	2609	CE	LYS	208	101.036	76.510	105.304	0.00	0.00	C
ATOM	2610	NZ	LYS	208	101.838	76.307	106.527	0.00	0.00	N
ATOM	2611	1HZ	LYS	208	101.282	76.576	107.351	1.00	0.00	H
ATOM	2612	2HZ	LYS	208	102.106	75.315	106.602	1.00	0.00	H
ATOM	2613	3HZ	LYS	208	102.687	76.889	106.482	1.00	0.00	H
ATOM	2614	H	LYS	208	103.435	76.102	99.387	0.00	0.00	H
ATOM	2615	HA	LYS	208	100.792	74.856	100.241	0.00	0.00	H
ATOM	2616	1HB	LYS	208	102.739	75.245	101.756	0.00	0.00	H
ATOM	2617	2HB	LYS	208	102.644	76.983	101.497	0.00	0.00	H
ATOM	2618	1HG	LYS	208	100.505	77.126	102.695	0.00	0.00	H
ATOM	2619	2HG	LYS	208	100.318	75.374	102.740	0.00	0.00	H
ATOM	2620	1HD	LYS	208	102.260	75.079	104.211	0.00	0.00	H
ATOM	2621	2HD	LYS	208	102.765	76.757	104.020	0.00	0.00	H
ATOM	2622	1HE	LYS	208	100.722	77.570	105.221	0.00	0.00	H
ATOM	2623	2HE	LYS	208	100.104	75.914	105.360	0.00	0.00	H
ATOM	2624	N	LYS	209	100.659	77.740	98.691	0.00	0.00	N
ATOM	2625	CA	LYS	209	99.705	78.666	97.997	0.00	0.00	C
ATOM	2626	C	LYS	209	99.374	78.284	96.498	0.00	0.00	C
ATOM	2627	O	LYS	209	98.226	78.420	96.065	0.00	0.00	O
ATOM	2628	CB	LYS	209	100.265	80.104	98.203	0.00	0.00	C
ATOM	2629	CG	LYS	209	99.332	81.261	97.765	0.00	0.00	C
ATOM	2630	CD	LYS	209	99.630	81.806	96.350	0.00	0.00	C
ATOM	2631	CE	LYS	209	98.518	82.713	95.793	0.00	0.00	C
ATOM	2632	NZ	LYS	209	97.422	81.903	95.221	0.00	0.00	N
ATOM	2633	1HZ	LYS	209	96.689	82.527	94.854	1.00	0.00	H
ATOM	2634	2HZ	LYS	209	97.789	81.319	94.457	1.00	0.00	H
ATOM	2635	3HZ	LYS	209	97.023	81.299	95.954	1.00	0.00	H
ATOM	2636	H	LYS	209	101.624	77.598	98.384	0.00	0.00	H
ATOM	2637	HA	LYS	209	98.723	78.635	98.513	0.00	0.00	H
ATOM	2638	1HB	LYS	209	100.457	80.245	99.286	0.00	0.00	H
ATOM	2639	2HB	LYS	209	101.263	80.211	97.735	0.00	0.00	H
ATOM	2640	1HG	LYS	209	98.273	80.948	97.853	0.00	0.00	H
ATOM	2641	2HG	LYS	209	99.430	82.095	98.485	0.00	0.00	H
ATOM	2642	1HD	LYS	209	100.572	82.388	96.396	0.00	0.00	H
ATOM	2643	2HD	LYS	209	99.846	80.986	95.638	0.00	0.00	H
ATOM	2644	1HE	LYS	209	98.125	83.390	96.578	0.00	0.00	H
ATOM	2645	2HE	LYS	209	98.924	83.383	95.009	0.00	0.00	H
ATOM	2646	N	THR	210	100.341	77.767	95.710	0.00	0.00	N
ATOM	2647	CA	THR	210	100.077	76.742	94.640	0.00	0.00	C
ATOM	2648	C	THR	210	99.851	77.267	93.177	0.00	0.00	C
ATOM	2649	O	THR	210	100.677	76.956	92.318	0.00	0.00	O
ATOM	2650	CB	THR	210	99.149	75.559	95.084	0.00	0.00	C
ATOM	2651	OG1	THR	210	99.601	75.041	96.330	0.00	0.00	O
ATOM	2652	CG2	THR	210	99.114	74.344	94.145	0.00	0.00	C
ATOM	2653	H	THR	210	101.215	77.717	96.237	0.00	0.00	H
ATOM	2654	HA	THR	210	101.060	76.239	94.553	0.00	0.00	H
ATOM	2655	HB	THR	210	98.116	75.943	95.207	0.00	0.00	H
ATOM	2656	HG1	THR	210	99.191	74.178	96.440	0.00	0.00	H
ATOM	2657	1HG2	THR	210	98.450	73.553	94.537	0.00	0.00	H
ATOM	2658	2HG2	THR	210	98.737	74.606	93.138	0.00	0.00	H
ATOM	2659	3HG2	THR	210	100.117	73.895	94.010	0.00	0.00	H
ATOM	2660	N	LEU	211	98.760	77.989	92.859	0.00	0.00	N
ATOM	2661	CA	LEU	211	98.390	78.383	91.462	0.00	0.00	C
ATOM	2662	C	LEU	211	98.152	79.921	91.268	0.00	0.00	C
ATOM	2663	O	LEU	211	97.299	80.524	91.926	0.00	0.00	O
ATOM	2664	CB	LEU	211	97.152	77.525	91.055	0.00	0.00	C
ATOM	2665	CG	LEU	211	96.653	77.648	89.589	0.00	0.00	C
ATOM	2666	CD1	LEU	211	97.684	77.137	88.570	0.00	0.00	C
ATOM	2667	CD2	LEU	211	95.344	76.862	89.403	0.00	0.00	C
ATOM	2668	H	LEU	211	98.174	78.215	93.673	1.00	0.00	H
ATOM	2669	HA	LEU	211	99.205	78.082	90.775	0.00	0.00	H
ATOM	2670	1HB	LEU	211	96.317	77.777	91.739	0.00	0.00	H
ATOM	2671	2HB	LEU	211	97.367	76.457	91.258	0.00	0.00	H
ATOM	2672	HG	LEU	211	96.437	78.714	89.370	0.00	0.00	H
ATOM	2673	1HD1	LEU	211	97.305	77.209	87.538	0.00	0.00	H
ATOM	2674	2HD1	LEU	211	98.623	77.717	88.593	0.00	0.00	H
ATOM	2675	3HD1	LEU	211	97.946	76.077	88.745	0.00	0.00	H
ATOM	2676	1HD2	LEU	211	94.944	76.959	88.377	0.00	0.00	H
ATOM	2677	2HD2	LEU	211	95.475	75.781	89.600	0.00	0.00	H
ATOM	2678	3HD2	LEU	211	94.551	77.222	90.084	0.00	0.00	H

ATOM	2679	N	CYS	212	98.844	80.530	90.287	0.00	0.00	N
ATOM	2680	CA	CYS	212	98.480	81.859	89.721	0.00	0.00	C
ATOM	2681	C	CYS	212	98.878	82.007	88.209	0.00	0.00	C
ATOM	2682	O	CYS	212	99.672	81.234	87.662	0.00	0.00	O
ATOM	2683	CB	CYS	212	99.121	82.952	90.615	0.00	0.00	C
ATOM	2684	SG	CYS	212	100.943	82.953	90.479	0.00	0.00	S
ATOM	2685	H	CYS	212	99.566	79.952	89.843	0.00	0.00	H
ATOM	2686	HA	CYS	212	97.378	81.976	89.772	0.00	0.00	H
ATOM	2687	1HB	CYS	212	98.834	82.823	91.677	0.00	0.00	H
ATOM	2688	2HB	CYS	212	98.750	83.954	90.330	0.00	0.00	H
ATOM	2689	HG	CYS	212	101.154	81.796	91.094	1.00	0.00	H
ATOM	2690	N	GLY	213	98.337	83.037	87.535	0.00	0.00	N
ATOM	2691	CA	GLY	213	98.800	83.453	86.181	0.00	0.00	C
ATOM	2692	C	GLY	213	97.663	83.738	85.183	0.00	0.00	C
ATOM	2693	O	GLY	213	96.866	84.657	85.383	0.00	0.00	O
ATOM	2694	H	GLY	213	97.707	83.619	88.099	0.00	0.00	H
ATOM	2695	1HA	GLY	213	99.534	82.740	85.752	0.00	0.00	H
ATOM	2696	2HA	GLY	213	99.374	84.392	86.282	0.00	0.00	H
ATOM	2697	N	THR	214	97.627	82.972	84.088	0.00	0.00	N
ATOM	2698	CA	THR	214	96.718	83.237	82.933	0.00	0.00	C
ATOM	2699	C	THR	214	96.128	81.867	82.441	0.00	0.00	C
ATOM	2700	O	THR	214	96.917	81.060	81.936	0.00	0.00	O
ATOM	2701	CB	THR	214	97.505	83.999	81.819	0.00	0.00	C
ATOM	2702	OG1	THR	214	97.923	85.263	82.313	0.00	0.00	O
ATOM	2703	CG2	THR	214	96.715	84.308	80.537	0.00	0.00	C
ATOM	2704	H	THR	214	98.341	82.239	84.062	0.00	0.00	H
ATOM	2705	HA	THR	214	95.895	83.909	83.235	0.00	0.00	H
ATOM	2706	HB	THR	214	98.407	83.413	81.557	0.00	0.00	H
ATOM	2707	HG1	THR	214	98.390	85.696	81.594	0.00	0.00	H
ATOM	2708	1HG2	THR	214	97.329	84.855	79.799	0.00	0.00	H
ATOM	2709	2HG2	THR	214	96.367	83.386	80.036	0.00	0.00	H
ATOM	2710	3HG2	THR	214	95.823	84.928	80.747	0.00	0.00	H
ATOM	2711	N	PRO	215	94.799	81.546	82.525	0.00	0.00	N
ATOM	2712	CA	PRO	215	94.254	80.205	82.148	0.00	0.00	C
ATOM	2713	CD	PRO	215	93.794	82.405	83.185	0.00	0.00	C
ATOM	2714	C	PRO	215	94.668	79.504	80.814	0.00	0.00	C
ATOM	2715	O	PRO	215	94.961	78.311	80.835	0.00	0.00	O
ATOM	2716	CB	PRO	215	92.735	80.418	82.290	0.00	0.00	C
ATOM	2717	CG	PRO	215	92.599	81.474	83.388	0.00	0.00	C
ATOM	2718	HA	PRO	215	94.580	79.510	82.945	0.00	0.00	H
ATOM	2719	1HD	PRO	215	93.527	83.261	82.535	0.00	0.00	H
ATOM	2720	2HD	PRO	215	94.140	82.814	84.156	0.00	0.00	H
ATOM	2721	1HB	PRO	215	92.203	79.478	82.536	0.00	0.00	H
ATOM	2722	2HB	PRO	215	92.296	80.791	81.344	0.00	0.00	H
ATOM	2723	1HG	PRO	215	92.652	80.997	84.386	0.00	0.00	H
ATOM	2724	2HG	PRO	215	91.637	82.017	83.344	0.00	0.00	H
ATOM	2725	N	ASN	216	94.745	80.230	79.689	1.00	0.00	N
ATOM	2726	CA	ASN	216	95.298	79.690	78.401	1.00	0.00	C
ATOM	2727	C	ASN	216	96.866	79.462	78.324	1.00	0.00	C
ATOM	2728	O	ASN	216	97.340	78.817	77.387	1.00	0.00	O
ATOM	2729	CB	ASN	216	94.840	80.631	77.244	1.00	0.00	C
ATOM	2730	CG	ASN	216	93.338	80.908	77.057	1.00	0.00	C
ATOM	2731	OD1	ASN	216	92.446	80.174	77.461	1.00	0.00	O
ATOM	2732	ND2	ASN	216	92.998	82.007	76.437	1.00	0.00	N
ATOM	2733	H	ASN	216	94.425	81.195	79.805	1.00	0.00	H
ATOM	2734	HA	ASN	216	94.848	78.695	78.209	1.00	0.00	H
ATOM	2735	1HB	ASN	216	95.381	81.591	77.334	1.00	0.00	H
ATOM	2736	2HB	ASN	216	95.186	80.193	76.288	1.00	0.00	H
ATOM	2737	1HD2	ASN	216	91.991	82.076	76.264	1.00	0.00	H
ATOM	2738	2HD2	ASN	216	93.751	82.524	75.978	1.00	0.00	H
ATOM	2739	N	TYR	217	97.665	80.015	79.256	0.00	0.00	N
ATOM	2740	CA	TYR	217	99.167	79.977	79.236	0.00	0.00	C
ATOM	2741	C	TYR	217	99.882	79.104	80.338	0.00	0.00	C
ATOM	2742	O	TYR	217	101.110	78.969	80.279	0.00	0.00	O
ATOM	2743	CB	TYR	217	99.650	81.465	79.294	0.00	0.00	C
ATOM	2744	CG	TYR	217	99.775	82.174	77.933	0.00	0.00	C
ATOM	2745	CD1	TYR	217	101.042	82.420	77.396	0.00	0.00	C
ATOM	2746	CE1	TYR	217	101.172	82.951	76.118	0.00	0.00	C
ATOM	2747	CZ	TYR	217	100.038	83.236	75.364	0.00	0.00	C
ATOM	2748	OH	TYR	217	100.171	83.611	74.059	0.00	0.00	O
ATOM	2749	CE2	TYR	217	98.772	83.046	75.907	0.00	0.00	C
ATOM	2750	CD2	TYR	217	98.639	82.526	77.193	0.00	0.00	C
ATOM	2751	H	TYR	217	97.212	80.500	80.044	1.00	0.00	H

ATOM	2752	HA	TYR	217	99.528	79.534	78.286	0.00	0.00	H
ATOM	2753	1HB	TYR	217	100.632	81.524	79.806	0.00	0.00	H
ATOM	2754	2HB	TYR	217	99.005	82.062	79.960	0.00	0.00	H
ATOM	2755	HD1	TYR	217	101.934	82.173	77.953	0.00	0.00	H
ATOM	2756	HE1	TYR	217	102.158	83.101	75.707	0.00	0.00	H
ATOM	2757	HH	TYR	217	101.054	83.350	73.772	0.00	0.00	H
ATOM	2758	HE2	TYR	217	97.896	83.266	75.315	0.00	0.00	H
ATOM	2759	HD2	TYR	217	97.654	82.353	77.596	0.00	0.00	H
ATOM	2760	N	ILE	218	99.176	78.544	81.339	1.00	0.00	N
ATOM	2761	CA	ILE	218	99.789	77.778	82.473	1.00	0.00	C
ATOM	2762	C	ILE	218	100.234	76.315	82.106	1.00	0.00	C
ATOM	2763	O	ILE	218	99.593	75.634	81.302	1.00	0.00	O
ATOM	2764	CB	ILE	218	98.852	77.782	83.741	1.00	0.00	C
ATOM	2765	CG1	ILE	218	97.441	77.159	83.512	1.00	0.00	C
ATOM	2766	CG2	ILE	218	98.755	79.177	84.408	1.00	0.00	C
ATOM	2767	CD1	ILE	218	96.717	76.713	84.792	1.00	0.00	C
ATOM	2768	H	ILE	218	98.162	78.681	81.261	1.00	0.00	H
ATOM	2769	HA	ILE	218	100.713	78.317	82.768	1.00	0.00	H
ATOM	2770	HB	ILE	218	99.357	77.140	84.489	1.00	0.00	H
ATOM	2771	1HG1	ILE	218	96.797	77.850	82.931	1.00	0.00	H
ATOM	2772	2HG1	ILE	218	97.535	76.264	82.866	1.00	0.00	H
ATOM	2773	2HG2	ILE	218	99.752	79.601	84.631	1.00	0.00	H
ATOM	2774	3HG2	ILE	218	98.227	79.903	83.765	1.00	0.00	H
ATOM	2775	1HG2	ILE	218	98.211	79.141	85.371	1.00	0.00	H
ATOM	2776	2HD1	ILE	218	97.360	76.074	85.427	1.00	0.00	H
ATOM	2777	3HD1	ILE	218	96.388	77.571	85.404	1.00	0.00	H
ATOM	2778	1HD1	ILE	218	95.818	76.116	84.556	1.00	0.00	H
ATOM	2779	N	ALA	219	101.320	75.825	82.731	0.00	0.00	N
ATOM	2780	CA	ALA	219	101.841	74.455	82.485	0.00	0.00	C
ATOM	2781	C	ALA	219	101.206	73.307	83.368	0.00	0.00	C
ATOM	2782	O	ALA	219	100.817	73.579	84.511	0.00	0.00	O
ATOM	2783	CB	ALA	219	103.364	74.552	82.711	0.00	0.00	C
ATOM	2784	H	ALA	219	101.770	76.471	83.382	0.00	0.00	H
ATOM	2785	HA	ALA	219	101.687	74.215	81.416	0.00	0.00	H
ATOM	2786	1HB	ALA	219	103.872	73.623	82.397	0.00	0.00	H
ATOM	2787	2HB	ALA	219	103.825	75.369	82.126	0.00	0.00	H
ATOM	2788	3HB	ALA	219	103.616	74.720	83.775	0.00	0.00	H
ATOM	2789	N	PRO	220	101.158	72.005	82.943	0.00	0.00	N
ATOM	2790	CA	PRO	220	100.659	70.877	83.791	0.00	0.00	C
ATOM	2791	CD	PRO	220	101.394	71.597	81.543	0.00	0.00	C
ATOM	2792	C	PRO	220	101.187	70.651	85.247	0.00	0.00	C
ATOM	2793	O	PRO	220	100.407	70.199	86.082	0.00	0.00	O
ATOM	2794	CB	PRO	220	100.904	69.656	82.883	0.00	0.00	C
ATOM	2795	CG	PRO	220	100.785	70.200	81.462	0.00	0.00	C
ATOM	2796	HA	PRO	220	99.562	71.009	83.886	0.00	0.00	H
ATOM	2797	1HD	PRO	220	102.476	71.581	81.306	0.00	0.00	H
ATOM	2798	2HD	PRO	220	100.898	72.264	80.814	0.00	0.00	H
ATOM	2799	1HB	PRO	220	100.186	68.836	83.080	0.00	0.00	H
ATOM	2800	2HB	PRO	220	101.916	69.231	83.038	0.00	0.00	H
ATOM	2801	1HG	PRO	220	99.721	70.265	81.158	0.00	0.00	H
ATOM	2802	2HG	PRO	220	101.288	69.563	80.711	0.00	0.00	H
ATOM	2803	N	GLU	221	102.455	70.966	85.580	0.00	0.00	N
ATOM	2804	CA	GLU	221	102.945	70.910	86.995	0.00	0.00	C
ATOM	2805	C	GLU	221	102.260	71.890	88.015	0.00	0.00	C
ATOM	2806	O	GLU	221	101.936	71.471	89.129	0.00	0.00	O
ATOM	2807	CB	GLU	221	104.487	71.081	87.071	0.00	0.00	C
ATOM	2808	CG	GLU	221	105.359	69.952	86.464	0.00	0.00	C
ATOM	2809	CD	GLU	221	106.798	70.025	86.972	0.00	0.00	C
ATOM	2810	OE1	GLU	221	107.633	70.826	86.560	0.00	0.00	O
ATOM	2811	OE2	GLU	221	107.020	69.153	87.992	0.00	0.00	O
ATOM	2812	H	GLU	221	102.987	71.365	84.803	0.00	0.00	H
ATOM	2813	HA	GLU	221	102.712	69.898	87.380	0.00	0.00	H
ATOM	2814	1HB	GLU	221	104.749	71.155	88.147	0.00	0.00	H
ATOM	2815	2HB	GLU	221	104.783	72.059	86.645	0.00	0.00	H
ATOM	2816	1HG	GLU	221	105.363	70.002	85.361	0.00	0.00	H
ATOM	2817	2HG	GLU	221	104.941	68.959	86.717	0.00	0.00	H
ATOM	2818	N	VAL	222	102.046	73.170	87.658	1.00	0.00	N
ATOM	2819	CA	VAL	222	101.206	74.108	88.480	1.00	0.00	C
ATOM	2820	C	VAL	222	99.684	73.725	88.570	1.00	0.00	C
ATOM	2821	O	VAL	222	99.093	73.815	89.649	1.00	0.00	O
ATOM	2822	CB	VAL	222	101.425	75.616	88.090	1.00	0.00	C
ATOM	2823	CG1	VAL	222	102.863	76.109	88.353	1.00	0.00	C
ATOM	2824	CG2	VAL	222	101.043	76.020	86.649	1.00	0.00	C

ATOM	2825	H	VAL	222	102.203	73.339	86.661	1.00	0.00	H
ATOM	2826	HA	VAL	222	101.561	74.024	89.528	1.00	0.00	H
ATOM	2827	HB	VAL	222	100.774	76.205	88.767	1.00	0.00	H
ATOM	2828	1HG1	VAL	222	103.609	75.553	87.759	1.00	0.00	H
ATOM	2829	2HG1	VAL	222	102.997	77.183	88.122	1.00	0.00	H
ATOM	2830	3HG1	VAL	222	103.135	75.982	89.416	1.00	0.00	H
ATOM	2831	2HG2	VAL	222	100.005	75.734	86.400	1.00	0.00	H
ATOM	2832	3HG2	VAL	222	101.111	77.114	86.497	1.00	0.00	H
ATOM	2833	1HG2	VAL	222	101.699	75.546	85.896	1.00	0.00	H
ATOM	2834	N	LEU	223	99.058	73.284	87.463	1.00	0.00	N
ATOM	2835	CA	LEU	223	97.660	72.767	87.463	1.00	0.00	C
ATOM	2836	C	LEU	223	97.419	71.428	88.252	1.00	0.00	C
ATOM	2837	O	LEU	223	96.535	71.382	89.110	1.00	0.00	O
ATOM	2838	CB	LEU	223	97.223	72.719	85.970	1.00	0.00	C
ATOM	2839	CG	LEU	223	95.765	72.282	85.690	1.00	0.00	C
ATOM	2840	CD1	LEU	223	94.728	73.218	86.333	1.00	0.00	C
ATOM	2841	CD2	LEU	223	95.530	72.202	84.175	1.00	0.00	C
ATOM	2842	H	LEU	223	99.671	73.215	86.643	1.00	0.00	H
ATOM	2843	HA	LEU	223	97.031	73.525	87.968	1.00	0.00	H
ATOM	2844	1HB	LEU	223	97.391	73.708	85.502	1.00	0.00	H
ATOM	2845	2HB	LEU	223	97.903	72.033	85.428	1.00	0.00	H
ATOM	2846	HG	LEU	223	95.616	71.263	86.104	1.00	0.00	H
ATOM	2847	2HD1	LEU	223	94.851	73.284	87.429	1.00	0.00	H
ATOM	2848	3HD1	LEU	223	94.782	74.249	85.935	1.00	0.00	H
ATOM	2849	1HD1	LEU	223	93.699	72.854	86.179	1.00	0.00	H
ATOM	2850	2HD2	LEU	223	95.604	73.188	83.680	1.00	0.00	H
ATOM	2851	3HD2	LEU	223	96.256	71.532	83.677	1.00	0.00	H
ATOM	2852	1HD2	LEU	223	94.532	71.792	83.951	1.00	0.00	H
ATOM	2853	N	SER	224	98.187	70.356	87.989	1.00	0.00	N
ATOM	2854	CA	SER	224	98.075	69.064	88.736	1.00	0.00	C
ATOM	2855	C	SER	224	98.658	68.999	90.199	1.00	0.00	C
ATOM	2856	O	SER	224	98.658	67.921	90.799	1.00	0.00	O
ATOM	2857	CB	SER	224	98.741	67.985	87.840	1.00	0.00	C
ATOM	2858	OG	SER	224	98.135	67.870	86.550	1.00	0.00	O
ATOM	2859	H	SER	224	98.879	70.476	87.238	1.00	0.00	H
ATOM	2860	HA	SER	224	97.005	68.795	88.832	1.00	0.00	H
ATOM	2861	1HB	SER	224	99.820	68.204	87.720	1.00	0.00	H
ATOM	2862	2HB	SER	224	98.702	66.998	88.340	1.00	0.00	H
ATOM	2863	HG	SER	224	97.378	67.267	86.625	1.00	0.00	H
ATOM	2864	N	LYS	225	99.135	70.118	90.782	1.00	0.00	N
ATOM	2865	CA	LYS	225	99.694	70.188	92.172	1.00	0.00	C
ATOM	2866	C	LYS	225	101.005	69.347	92.400	1.00	0.00	C
ATOM	2867	O	LYS	225	101.078	68.465	93.259	1.00	0.00	O
ATOM	2868	CB	LYS	225	98.586	69.988	93.255	1.00	0.00	C
ATOM	2869	CG	LYS	225	97.368	70.940	93.162	1.00	0.00	C
ATOM	2870	CD	LYS	225	96.400	70.792	94.350	1.00	0.00	C
ATOM	2871	CE	LYS	225	95.179	71.713	94.203	1.00	0.00	C
ATOM	2872	NZ	LYS	225	94.285	71.539	95.364	1.00	0.00	N
ATOM	2873	1HZ	LYS	225	93.467	72.156	95.264	1.00	0.00	H
ATOM	2874	2HZ	LYS	225	93.970	70.559	95.412	1.00	0.00	H
ATOM	2875	3HZ	LYS	225	94.792	71.779	96.228	1.00	0.00	H
ATOM	2876	H	LYS	225	98.995	70.950	90.199	1.00	0.00	H
ATOM	2877	HA	LYS	225	100.027	71.236	92.303	1.00	0.00	H
ATOM	2878	1HB	LYS	225	98.236	68.938	93.219	1.00	0.00	H
ATOM	2879	2HB	LYS	225	99.054	70.093	94.253	1.00	0.00	H
ATOM	2880	1HG	LYS	225	97.711	71.987	93.077	1.00	0.00	H
ATOM	2881	2HG	LYS	225	96.824	70.743	92.216	1.00	0.00	H
ATOM	2882	1HD	LYS	225	96.066	69.738	94.425	1.00	0.00	H
ATOM	2883	2HD	LYS	225	96.934	71.007	95.295	1.00	0.00	H
ATOM	2884	1HE	LYS	225	95.494	72.772	94.114	1.00	0.00	H
ATOM	2885	2HE	LYS	225	94.630	71.476	93.268	1.00	0.00	H
ATOM	2886	N	LYS	226	102.052	69.648	91.613	0.00	0.00	N
ATOM	2887	CA	LYS	226	103.328	68.872	91.587	0.00	0.00	C
ATOM	2888	C	LYS	226	104.564	69.752	92.003	0.00	0.00	C
ATOM	2889	O	LYS	226	104.453	70.949	92.291	0.00	0.00	O
ATOM	2890	CB	LYS	226	103.451	68.283	90.144	0.00	0.00	C
ATOM	2891	CG	LYS	226	102.481	67.124	89.805	0.00	0.00	C
ATOM	2892	CD	LYS	226	102.522	66.736	88.315	0.00	0.00	C
ATOM	2893	CE	LYS	226	101.637	65.515	88.023	0.00	0.00	C
ATOM	2894	NZ	LYS	226	101.527	65.311	86.566	0.00	0.00	N
ATOM	2895	1HZ	LYS	226	100.932	64.491	86.378	1.00	0.00	H
ATOM	2896	2HZ	LYS	226	101.107	66.146	86.133	1.00	0.00	H
ATOM	2897	3HZ	LYS	226	102.464	65.153	86.169	1.00	0.00	H

ATOM	2898	H	LYS	226	101.835	70.349	90.892	0.00	0.00	H
ATOM	2899	HA	LYS	226	103.295	68.031	92.309	0.00	0.00	H
ATOM	2900	1HB	LYS	226	104.478	67.911	89.973	0.00	0.00	H
ATOM	2901	2HB	LYS	226	103.337	69.102	89.410	0.00	0.00	H
ATOM	2902	1HG	LYS	226	101.442	67.407	90.074	0.00	0.00	H
ATOM	2903	2HG	LYS	226	102.712	66.247	90.442	0.00	0.00	H
ATOM	2904	1HD	LYS	226	103.564	66.527	88.001	0.00	0.00	H
ATOM	2905	2HD	LYS	226	102.191	67.603	87.712	0.00	0.00	H
ATOM	2906	1HE	LYS	226	100.625	65.645	88.456	0.00	0.00	H
ATOM	2907	2HE	LYS	226	102.050	64.607	88.504	0.00	0.00	H
ATOM	2908	N	GLY	227	105.779	69.164	92.013	0.00	0.00	N
ATOM	2909	CA	GLY	227	107.043	69.942	92.196	0.00	0.00	C
ATOM	2910	C	GLY	227	107.474	70.781	90.969	0.00	0.00	C
ATOM	2911	O	GLY	227	108.252	70.317	90.129	0.00	0.00	O
ATOM	2912	H	GLY	227	105.763	68.170	91.767	0.00	0.00	H
ATOM	2913	1HA	GLY	227	107.867	69.245	92.430	0.00	0.00	H
ATOM	2914	2HA	GLY	227	106.975	70.593	93.090	0.00	0.00	H
ATOM	2915	N	HIS	228	106.938	72.001	90.862	1.00	0.00	N
ATOM	2916	CA	HIS	228	107.134	72.882	89.682	1.00	0.00	C
ATOM	2917	C	HIS	228	108.488	73.673	89.671	1.00	0.00	C
ATOM	2918	O	HIS	228	109.095	73.931	90.713	1.00	0.00	O
ATOM	2919	CB	HIS	228	105.849	73.745	89.522	1.00	0.00	C
ATOM	2920	CG	HIS	228	105.638	74.923	90.476	1.00	0.00	C
ATOM	2921	ND1	HIS	228	104.839	74.852	91.605	1.00	0.00	N
ATOM	2922	CE1	HIS	228	104.822	76.176	91.952	1.00	0.00	C
ATOM	2923	NE2	HIS	228	105.504	77.090	91.195	1.00	0.00	N
ATOM	2924	CD2	HIS	228	106.028	76.252	90.228	1.00	0.00	C
ATOM	2925	H	HIS	228	106.269	72.229	91.611	1.00	0.00	H
ATOM	2926	HA	HIS	228	107.156	72.227	88.789	1.00	0.00	H
ATOM	2927	1HB	HIS	228	105.814	74.126	88.490	1.00	0.00	H
ATOM	2928	2HB	HIS	228	104.952	73.095	89.578	1.00	0.00	H
ATOM	2929	HE1	HIS	228	104.223	76.496	92.796	1.00	0.00	H
ATOM	2930	HE2	HIS	228	105.433	78.113	91.204	1.00	0.00	H
ATOM	2931	HD2	HIS	228	106.583	76.576	89.357	1.00	0.00	H
ATOM	2932	N	SER	229	108.982	74.034	88.477	1.00	0.00	N
ATOM	2933	CA	SER	229	110.344	74.627	88.307	1.00	0.00	C
ATOM	2934	C	SER	229	110.413	75.767	87.228	1.00	0.00	C
ATOM	2935	O	SER	229	109.414	76.160	86.618	1.00	0.00	O
ATOM	2936	CB	SER	229	111.307	73.436	88.019	1.00	0.00	C
ATOM	2937	OG	SER	229	111.082	72.858	86.728	1.00	0.00	O
ATOM	2938	H	SER	229	108.401	73.777	87.675	1.00	0.00	H
ATOM	2939	HA	SER	229	110.667	75.107	89.254	1.00	0.00	H
ATOM	2940	1HB	SER	229	112.359	73.774	88.078	1.00	0.00	H
ATOM	2941	2HB	SER	229	111.226	72.659	88.807	1.00	0.00	H
ATOM	2942	HG	SER	229	110.404	72.178	86.829	1.00	0.00	H
ATOM	2943	N	PHE	230	111.629	76.267	86.950	1.00	0.00	N
ATOM	2944	CA	PHE	230	111.937	77.099	85.741	1.00	0.00	C
ATOM	2945	C	PHE	230	111.471	76.593	84.316	1.00	0.00	C
ATOM	2946	O	PHE	230	111.222	77.406	83.423	1.00	0.00	O
ATOM	2947	CB	PHE	230	113.452	77.459	85.816	1.00	0.00	C
ATOM	2948	CG	PHE	230	114.486	76.333	85.620	1.00	0.00	C
ATOM	2949	CD1	PHE	230	114.974	76.051	84.343	1.00	0.00	C
ATOM	2950	CE1	PHE	230	115.897	75.025	84.148	1.00	0.00	C
ATOM	2951	CZ	PHE	230	116.347	74.284	85.237	1.00	0.00	C
ATOM	2952	CE2	PHE	230	115.881	74.568	86.518	1.00	0.00	C
ATOM	2953	CD2	PHE	230	114.956	75.593	86.710	1.00	0.00	C
ATOM	2954	H	PHE	230	112.386	75.821	87.479	1.00	0.00	H
ATOM	2955	HA	PHE	230	111.391	78.053	85.871	1.00	0.00	H
ATOM	2956	1HB	PHE	230	113.651	78.247	85.071	1.00	0.00	H
ATOM	2957	2HB	PHE	230	113.669	77.979	86.769	1.00	0.00	H
ATOM	2958	HD1	PHE	230	114.632	76.633	83.501	1.00	0.00	H
ATOM	2959	HE1	PHE	230	116.265	74.805	83.156	1.00	0.00	H
ATOM	2960	HZ	PHE	230	117.066	73.490	85.087	1.00	0.00	H
ATOM	2961	HE2	PHE	230	116.243	73.999	87.361	1.00	0.00	H
ATOM	2962	HD2	PHE	230	114.613	75.812	87.710	1.00	0.00	H
ATOM	2963	N	GLU	231	111.292	75.272	84.131	1.00	0.00	N
ATOM	2964	CA	GLU	231	110.562	74.677	82.969	1.00	0.00	C
ATOM	2965	C	GLU	231	109.060	75.098	82.737	1.00	0.00	C
ATOM	2966	O	GLU	231	108.584	75.005	81.604	1.00	0.00	O
ATOM	2967	CB	GLU	231	110.656	73.133	83.100	1.00	0.00	C
ATOM	2968	CG	GLU	231	112.078	72.518	83.008	1.00	0.00	C
ATOM	2969	CD	GLU	231	112.065	70.999	82.925	1.00	0.00	C
ATOM	2970	OE1	GLU	231	112.137	70.254	83.897	1.00	0.00	O

ATOM	2971	OE2	GLU	231	111.937	70.573	81.644	1.00	0.00	O
ATOM	2972	H	GLU	231	111.571	74.703	84.940	1.00	0.00	H
ATOM	2973	HA	GLU	231	111.097	74.967	82.041	1.00	0.00	H
ATOM	2974	1HB	GLU	231	110.167	72.799	84.038	1.00	0.00	H
ATOM	2975	2HB	GLU	231	110.045	72.676	82.297	1.00	0.00	H
ATOM	2976	1HG	GLU	231	112.608	72.908	82.120	1.00	0.00	H
ATOM	2977	2HG	GLU	231	112.696	72.813	83.876	1.00	0.00	H
ATOM	2978	N	VAL	232	108.315	75.563	83.762	0.00	0.00	N
ATOM	2979	CA	VAL	232	106.975	76.233	83.587	0.00	0.00	C
ATOM	2980	C	VAL	232	106.973	77.440	82.572	0.00	0.00	C
ATOM	2981	O	VAL	232	106.066	77.540	81.743	0.00	0.00	O
ATOM	2982	CB	VAL	232	106.397	76.618	85.002	0.00	0.00	C
ATOM	2983	CG1	VAL	232	105.069	77.417	84.983	0.00	0.00	C
ATOM	2984	CG2	VAL	232	106.142	75.406	85.927	0.00	0.00	C
ATOM	2985	H	VAL	232	108.833	75.616	84.649	0.00	0.00	H
ATOM	2986	HA	VAL	232	106.286	75.487	83.145	0.00	0.00	H
ATOM	2987	HB	VAL	232	107.150	77.263	85.501	0.00	0.00	H
ATOM	2988	1HG1	VAL	232	104.717	77.675	86.001	0.00	0.00	H
ATOM	2989	2HG1	VAL	232	105.171	78.380	84.448	0.00	0.00	H
ATOM	2990	3HG1	VAL	232	104.250	76.866	84.487	0.00	0.00	H
ATOM	2991	1HG2	VAL	232	105.825	75.734	86.933	0.00	0.00	H
ATOM	2992	2HG2	VAL	232	105.361	74.727	85.535	0.00	0.00	H
ATOM	2993	3HG2	VAL	232	107.054	74.800	86.076	0.00	0.00	H
ATOM	2994	N	ASP	233	107.988	78.323	82.624	0.00	0.00	N
ATOM	2995	CA	ASP	233	108.152	79.450	81.659	0.00	0.00	C
ATOM	2996	C	ASP	233	108.270	79.073	80.140	0.00	0.00	C
ATOM	2997	O	ASP	233	107.709	79.791	79.312	0.00	0.00	O
ATOM	2998	CB	ASP	233	109.365	80.306	82.112	0.00	0.00	C
ATOM	2999	CG	ASP	233	109.178	81.054	83.429	0.00	0.00	C
ATOM	3000	OD1	ASP	233	108.462	82.039	83.552	0.00	0.00	O
ATOM	3001	OD2	ASP	233	109.888	80.506	84.452	0.00	0.00	O
ATOM	3002	H	ASP	233	108.728	78.048	83.281	0.00	0.00	H
ATOM	3003	HA	ASP	233	107.242	80.084	81.725	0.00	0.00	H
ATOM	3004	1HB	ASP	233	109.579	81.077	81.350	0.00	0.00	H
ATOM	3005	2HB	ASP	233	110.280	79.686	82.156	0.00	0.00	H
ATOM	3006	N	VAL	234	108.966	77.984	79.753	1.00	0.00	N
ATOM	3007	CA	VAL	234	109.051	77.551	78.315	1.00	0.00	C
ATOM	3008	C	VAL	234	107.716	77.024	77.672	1.00	0.00	C
ATOM	3009	O	VAL	234	107.491	77.285	76.490	1.00	0.00	O
ATOM	3010	CB	VAL	234	110.287	76.640	77.996	1.00	0.00	C
ATOM	3011	CG1	VAL	234	111.637	77.212	78.478	1.00	0.00	C
ATOM	3012	CG2	VAL	234	110.179	75.177	78.463	1.00	0.00	C
ATOM	3013	H	VAL	234	109.295	77.390	80.522	1.00	0.00	H
ATOM	3014	HA	VAL	234	109.256	78.472	77.736	1.00	0.00	H
ATOM	3015	HB	VAL	234	110.352	76.595	76.889	1.00	0.00	H
ATOM	3016	1HG1	VAL	234	111.830	78.217	78.064	1.00	0.00	H
ATOM	3017	2HG1	VAL	234	111.679	77.294	79.581	1.00	0.00	H
ATOM	3018	3HG1	VAL	234	112.485	76.569	78.180	1.00	0.00	H
ATOM	3019	2HG2	VAL	234	109.275	74.691	78.054	1.00	0.00	H
ATOM	3020	3HG2	VAL	234	111.032	74.567	78.108	1.00	0.00	H
ATOM	3021	1HG2	VAL	234	110.144	75.080	79.563	1.00	0.00	H
ATOM	3022	N	TRP	235	106.805	76.370	78.426	0.00	0.00	N
ATOM	3023	CA	TRP	235	105.377	76.190	78.008	0.00	0.00	C
ATOM	3024	C	TRP	235	104.631	77.524	77.617	0.00	0.00	C
ATOM	3025	O	TRP	235	104.044	77.605	76.537	0.00	0.00	O
ATOM	3026	CB	TRP	235	104.678	75.370	79.134	0.00	0.00	C
ATOM	3027	CG	TRP	235	103.237	74.907	78.840	0.00	0.00	C
ATOM	3028	CD1	TRP	235	102.087	75.732	78.847	0.00	0.00	C
ATOM	3029	NE1	TRP	235	100.919	75.016	78.528	0.00	0.00	N
ATOM	3030	CE2	TRP	235	101.363	73.721	78.340	0.00	0.00	C
ATOM	3031	CD2	TRP	235	102.767	73.636	78.544	0.00	0.00	C
ATOM	3032	CE3	TRP	235	103.427	72.383	78.450	0.00	0.00	C
ATOM	3033	CZ3	TRP	235	102.666	71.256	78.137	0.00	0.00	C
ATOM	3034	CH2	TRP	235	101.286	71.342	77.920	0.00	0.00	C
ATOM	3035	CZ2	TRP	235	100.618	72.563	78.027	0.00	0.00	C
ATOM	3036	H	TRP	235	107.125	76.193	79.384	0.00	0.00	H
ATOM	3037	HA	TRP	235	105.383	75.559	77.096	0.00	0.00	H
ATOM	3038	1HB	TRP	235	104.675	75.961	80.068	0.00	0.00	H
ATOM	3039	2HB	TRP	235	105.288	74.475	79.371	0.00	0.00	H
ATOM	3040	HD1	TRP	235	102.100	76.787	79.085	0.00	0.00	H
ATOM	3041	HE1	TRP	235	99.945	75.330	78.617	0.00	0.00	H
ATOM	3042	HE3	TRP	235	104.496	72.298	78.604	0.00	0.00	H
ATOM	3043	HZ3	TRP	235	103.151	70.298	78.052	0.00	0.00	H

ATOM	3044	HH2	TRP	235	100.726	70.451	77.675	0.00	0.00	H
ATOM	3045	HZ2	TRP	235	99.552	72.617	77.872	0.00	0.00	H
ATOM	3046	N	SER	236	104.693	78.574	78.457	1.00	0.00	N
ATOM	3047	CA	SER	236	104.260	79.951	78.074	1.00	0.00	C
ATOM	3048	C	SER	236	105.007	80.630	76.859	1.00	0.00	C
ATOM	3049	O	SER	236	104.369	81.372	76.112	1.00	0.00	O
ATOM	3050	CB	SER	236	104.309	80.831	79.347	1.00	0.00	C
ATOM	3051	OG	SER	236	103.493	80.340	80.418	1.00	0.00	O
ATOM	3052	H	SER	236	105.222	78.388	79.317	1.00	0.00	H
ATOM	3053	HA	SER	236	103.196	79.893	77.768	1.00	0.00	H
ATOM	3054	1HB	SER	236	105.351	80.918	79.709	1.00	0.00	H
ATOM	3055	2HB	SER	236	103.998	81.867	79.110	1.00	0.00	H
ATOM	3056	HG	SER	236	102.778	79.795	80.055	1.00	0.00	H
ATOM	3057	N	ILE	237	106.309	80.357	76.616	1.00	0.00	N
ATOM	3058	CA	ILE	237	107.003	80.705	75.321	1.00	0.00	C
ATOM	3059	C	ILE	237	106.456	79.903	74.072	1.00	0.00	C
ATOM	3060	O	ILE	237	106.248	80.500	73.014	1.00	0.00	O
ATOM	3061	CB	ILE	237	108.578	80.663	75.438	1.00	0.00	C
ATOM	3062	CG1	ILE	237	109.157	81.505	76.618	1.00	0.00	C
ATOM	3063	CG2	ILE	237	109.275	81.142	74.129	1.00	0.00	C
ATOM	3064	CD1	ILE	237	110.646	81.287	76.949	1.00	0.00	C
ATOM	3065	H	ILE	237	106.740	79.761	77.333	1.00	0.00	H
ATOM	3066	HA	ILE	237	106.758	81.763	75.117	1.00	0.00	H
ATOM	3067	HB	ILE	237	108.860	79.603	75.604	1.00	0.00	H
ATOM	3068	1HG1	ILE	237	108.966	82.579	76.437	1.00	0.00	H
ATOM	3069	2HG1	ILE	237	108.591	81.285	77.540	1.00	0.00	H
ATOM	3070	2HG2	ILE	237	108.960	80.560	73.244	1.00	0.00	H
ATOM	3071	3HG2	ILE	237	109.062	82.205	73.906	1.00	0.00	H
ATOM	3072	1HG2	ILE	237	110.374	81.034	74.173	1.00	0.00	H
ATOM	3073	2HD1	ILE	237	110.884	80.218	77.100	1.00	0.00	H
ATOM	3074	3HD1	ILE	237	111.312	81.668	76.152	1.00	0.00	H
ATOM	3075	1HD1	ILE	237	110.933	81.818	77.875	1.00	0.00	H
ATOM	3076	N	GLY	238	106.200	78.583	74.167	0.00	0.00	N
ATOM	3077	CA	GLY	238	105.387	77.841	73.149	0.00	0.00	C
ATOM	3078	C	GLY	238	103.976	76.385	72.795	0.00	0.00	C
ATOM	3079	O	GLY	238	103.633	78.481	71.615	0.00	0.00	O
ATOM	3080	H	GLY	238	106.452	78.180	75.081	0.00	0.00	H
ATOM	3081	1HA	GLY	238	105.261	76.799	73.491	0.00	0.00	H
ATOM	3082	2HA	GLY	238	105.967	77.757	72.212	0.00	0.00	H
ATOM	3083	N	CYS	239	103.189	78.784	73.803	1.00	0.00	N
ATOM	3084	CA	CYS	239	101.955	79.588	73.598	1.00	0.00	C
ATOM	3085	C	CYS	239	102.130	81.037	73.017	1.00	0.00	C
ATOM	3086	O	CYS	239	101.320	81.424	72.177	1.00	0.00	O
ATOM	3087	CB	CYS	239	101.175	79.555	74.929	1.00	0.00	C
ATOM	3088	SG	CYS	239	100.684	77.847	75.353	1.00	0.00	S
ATOM	3089	H	CYS	239	103.559	78.560	74.737	1.00	0.00	H
ATOM	3090	HA	CYS	239	101.333	79.056	72.854	1.00	0.00	H
ATOM	3091	1HB	CYS	239	101.770	79.984	75.756	1.00	0.00	H
ATOM	3092	2HB	CYS	239	100.257	80.168	74.857	1.00	0.00	H
ATOM	3093	HG	CYS	239	99.879	78.149	76.369	1.00	0.00	H
ATOM	3094	N	ILE	240	103.144	81.846	73.401	1.00	0.00	N
ATOM	3095	CA	ILE	240	103.446	83.157	72.720	1.00	0.00	C
ATOM	3096	C	ILE	240	103.857	83.041	71.205	1.00	0.00	C
ATOM	3097	O	ILE	240	103.322	83.776	70.376	1.00	0.00	O
ATOM	3098	CB	ILE	240	104.363	84.074	73.623	1.00	0.00	C
ATOM	3099	CG1	ILE	240	104.030	85.592	73.537	1.00	0.00	C
ATOM	3100	CG2	ILE	240	105.884	83.930	73.375	1.00	0.00	C
ATOM	3101	CD1	ILE	240	102.718	86.012	74.219	1.00	0.00	C
ATOM	3102	H	ILE	240	103.768	81.425	74.103	1.00	0.00	H
ATOM	3103	HA	ILE	240	102.475	83.683	72.661	1.00	0.00	H
ATOM	3104	HB	ILE	240	104.204	83.784	74.683	1.00	0.00	H
ATOM	3105	1HG1	ILE	240	104.839	86.186	74.008	1.00	0.00	H
ATOM	3106	2HG1	ILE	240	104.027	85.921	72.479	1.00	0.00	H
ATOM	3107	2HG2	ILE	240	106.194	82.878	73.307	1.00	0.00	H
ATOM	3108	3HG2	ILE	240	106.204	84.406	72.428	1.00	0.00	H
ATOM	3109	1HG2	ILE	240	106.480	84.382	74.189	1.00	0.00	H
ATOM	3110	2HD1	ILE	240	101.825	85.624	73.696	1.00	0.00	H
ATOM	3111	3HD1	ILE	240	102.667	85.675	75.270	1.00	0.00	H
ATOM	3112	1HD1	ILE	240	102.619	87.114	74.233	1.00	0.00	H
ATOM	3113	N	MET	241	104.735	82.087	70.837	1.00	0.00	N
ATOM	3114	CA	MET	241	104.976	81.681	69.418	1.00	0.00	C
ATOM	3115	C	MET	241	103.699	81.313	68.578	1.00	0.00	C
ATOM	3116	O	MET	241	103.509	81.859	67.490	1.00	0.00	O

ATOM	3117	CB	MET	241	106.015	80.527	69.488	1.00	0.00	C
ATOM	3118	CG	MET	241	106.567	80.031	68.129	1.00	0.00	C
ATOM	3119	SD	MET	241	107.621	78.555	68.239	1.00	0.00	S
ATOM	3120	CE	MET	241	108.499	78.673	69.810	1.00	0.00	C
ATOM	3121	H	MET	241	105.091	81.530	71.626	1.00	0.00	H
ATOM	3122	HA	MET	241	105.453	82.535	68.899	1.00	0.00	H
ATOM	3123	1HB	MET	241	106.874	80.850	70.110	1.00	0.00	H
ATOM	3124	2HB	MET	241	105.577	79.664	70.029	1.00	0.00	H
ATOM	3125	1HG	MET	241	105.735	79.767	67.450	1.00	0.00	H
ATOM	3126	2HG	MET	241	107.116	80.834	67.606	1.00	0.00	H
ATOM	3127	1HE	MET	241	109.111	79.588	69.866	1.00	0.00	H
ATOM	3128	3HE	MET	241	107.793	78.671	70.659	1.00	0.00	H
ATOM	3129	2HE	MET	241	109.169	77.807	69.936	1.00	0.00	H
ATOM	3130	N	TYR	242	102.832	80.420	69.086	0.00	0.00	N
ATOM	3131	CA	TYR	242	101.524	80.095	68.447	0.00	0.00	C
ATOM	3132	C	TYR	242	100.518	81.301	68.359	0.00	0.00	C
ATOM	3133	O	TYR	242	100.074	81.616	67.254	0.00	0.00	O
ATOM	3134	CB	TYR	242	100.977	78.843	69.192	0.00	0.00	C
ATOM	3135	CG	TYR	242	99.848	78.067	68.487	0.00	0.00	C
ATOM	3136	CD1	TYR	242	98.549	78.587	68.430	0.00	0.00	C
ATOM	3137	CE1	TYR	242	97.505	77.821	67.920	0.00	0.00	C
ATOM	3138	CZ	TYR	242	97.747	76.525	67.476	0.00	0.00	C
ATOM	3139	OH	TYR	242	96.709	75.742	67.055	0.00	0.00	O
ATOM	3140	CE2	TYR	242	99.037	76.005	67.506	0.00	0.00	C
ATOM	3141	CD2	TYR	242	100.086	76.773	68.008	0.00	0.00	C
ATOM	3142	H	TYR	242	103.082	79.937	69.961	1.00	0.00	H
ATOM	3143	HA	TYR	242	101.733	79.791	67.401	0.00	0.00	H
ATOM	3144	1HB	TYR	242	100.640	79.136	70.204	0.00	0.00	H
ATOM	3145	2HB	TYR	242	101.809	78.139	69.399	0.00	0.00	H
ATOM	3146	HD1	TYR	242	98.325	79.574	68.813	0.00	0.00	H
ATOM	3147	HE1	TYR	242	96.504	78.227	67.911	0.00	0.00	H
ATOM	3148	HH	TYR	242	95.880	76.166	67.285	0.00	0.00	H
ATOM	3149	HE2	TYR	242	99.213	74.992	67.173	0.00	0.00	H
ATOM	3150	HD2	TYR	242	101.076	76.342	68.058	0.00	0.00	H
ATOM	3151	N	THR	243	100.184	81.981	69.478	1.00	0.00	N
ATOM	3152	CA	THR	243	99.285	83.185	69.481	1.00	0.00	C
ATOM	3153	C	THR	243	99.713	84.342	68.514	1.00	0.00	C
ATOM	3154	O	THR	243	98.888	84.807	67.726	1.00	0.00	O
ATOM	3155	CB	THR	243	99.090	83.743	70.932	1.00	0.00	C
ATOM	3156	OG1	THR	243	98.832	82.718	71.884	1.00	0.00	O
ATOM	3157	CG2	THR	243	97.910	84.721	71.059	1.00	0.00	C
ATOM	3158	H	THR	243	100.655	81.660	70.333	1.00	0.00	H
ATOM	3159	HA	THR	243	98.293	82.839	69.129	1.00	0.00	H
ATOM	3160	HB	THR	243	100.024	84.260	71.238	1.00	0.00	H
ATOM	3161	HG1	THR	243	99.139	83.061	72.734	1.00	0.00	H
ATOM	3162	1HG2	THR	243	97.704	85.005	72.105	1.00	0.00	H
ATOM	3163	2HG2	THR	243	98.085	85.655	70.491	1.00	0.00	H
ATOM	3164	3HG2	THR	243	96.979	84.281	70.658	1.00	0.00	H
ATOM	3165	N	LEU	244	100.985	84.781	68.545	1.00	0.00	N
ATOM	3166	CA	LEU	244	101.545	85.737	67.545	1.00	0.00	C
ATOM	3167	C	LEU	244	101.478	85.258	66.049	1.00	0.00	C
ATOM	3168	O	LEU	244	101.053	86.030	65.189	1.00	0.00	O
ATOM	3169	CB	LEU	244	102.996	86.108	67.971	1.00	0.00	C
ATOM	3170	CG	LEU	244	103.197	86.828	69.336	1.00	0.00	C
ATOM	3171	CD1	LEU	244	104.693	86.857	69.681	1.00	0.00	C
ATOM	3172	CD2	LEU	244	102.634	88.258	69.364	1.00	0.00	C
ATOM	3173	H	LEU	244	101.595	84.257	69.185	1.00	0.00	H
ATOM	3174	HA	LEU	244	100.944	86.664	67.584	1.00	0.00	H
ATOM	3175	1HB	LEU	244	103.598	85.177	67.962	1.00	0.00	H
ATOM	3176	2HB	LEU	244	103.453	86.732	67.179	1.00	0.00	H
ATOM	3177	HG	LEU	244	102.682	86.247	70.127	1.00	0.00	H
ATOM	3178	2HD1	LEU	244	105.106	85.835	69.783	1.00	0.00	H
ATOM	3179	3HD1	LEU	244	105.282	87.366	68.897	1.00	0.00	H
ATOM	3180	1HD1	LEU	244	104.891	87.376	70.636	1.00	0.00	H
ATOM	3181	2HD2	LEU	244	103.144	88.924	68.647	1.00	0.00	H
ATOM	3182	3HD2	LEU	244	101.554	88.286	69.124	1.00	0.00	H
ATOM	3183	1HD2	LEU	244	102.744	88.721	70.362	1.00	0.00	H
ATOM	3184	N	LEU	245	101.858	84.002	65.739	1.00	0.00	N
ATOM	3185	CA	LEU	245	101.796	83.446	64.357	1.00	0.00	C
ATOM	3186	C	LEU	245	100.365	83.227	63.747	1.00	0.00	C
ATOM	3187	O	LEU	245	100.130	83.686	62.629	1.00	0.00	O
ATOM	3188	CB	LEU	245	102.732	82.203	64.331	1.00	0.00	C
ATOM	3189	CG	LEU	245	102.919	81.454	62.985	1.00	0.00	C

ATOM	3190	CD1	LEU	245	103.344	82.362	61.820	1.00	0.00	C
ATOM	3191	CD2	LEU	245	103.963	80.340	63.152	1.00	0.00	C
ATOM	3192	H	LEU	245	102.133	83.433	66.548	1.00	0.00	H
ATOM	3193	HA	LEU	245	102.271	84.194	63.697	1.00	0.00	H
ATOM	3194	1HB	LEU	245	103.730	82.513	64.700	1.00	0.00	H
ATOM	3195	2HB	LEU	245	102.371	81.475	65.084	1.00	0.00	H
ATOM	3196	HG	LEU	245	101.953	80.980	62.714	1.00	0.00	H
ATOM	3197	2HD1	LEU	245	102.592	83.146	61.614	1.00	0.00	H
ATOM	3198	3HD1	LEU	245	104.301	82.881	62.016	1.00	0.00	H
ATOM	3199	1HD1	LEU	245	103.446	81.789	60.880	1.00	0.00	H
ATOM	3200	2HD2	LEU	245	104.967	80.740	63.387	1.00	0.00	H
ATOM	3201	3HD2	LEU	245	103.690	79.650	63.972	1.00	0.00	H
ATOM	3202	1HD2	LEU	245	104.055	79.729	62.234	1.00	0.00	H
ATOM	3203	N	VAL	246	99.420	82.532	64.412	1.00	0.00	N
ATOM	3204	CA	VAL	246	98.018	82.373	63.887	1.00	0.00	C
ATOM	3205	C	VAL	246	97.012	83.542	64.197	1.00	0.00	C
ATOM	3206	O	VAL	246	96.113	83.787	63.387	1.00	0.00	O
ATOM	3207	CB	VAL	246	97.466	80.939	64.220	1.00	0.00	C
ATOM	3208	CG1	VAL	246	97.060	80.705	65.691	1.00	0.00	C
ATOM	3209	CG2	VAL	246	96.256	80.541	63.340	1.00	0.00	C
ATOM	3210	H	VAL	246	99.698	82.253	65.364	1.00	0.00	H
ATOM	3211	HA	VAL	246	98.082	82.391	62.781	1.00	0.00	H
ATOM	3212	HB	VAL	246	98.274	80.217	63.987	1.00	0.00	H
ATOM	3213	1HG1	VAL	246	96.219	81.348	66.008	1.00	0.00	H
ATOM	3214	2HG1	VAL	246	96.751	79.661	65.873	1.00	0.00	H
ATOM	3215	3HG1	VAL	246	97.889	80.912	66.389	1.00	0.00	H
ATOM	3216	2HG2	VAL	246	96.503	80.566	62.265	1.00	0.00	H
ATOM	3217	3HG2	VAL	246	95.894	79.519	63.559	1.00	0.00	H
ATOM	3218	1HG2	VAL	246	95.393	81.219	63.488	1.00	0.00	H
ATOM	3219	N	GLY	247	97.099	84.206	65.360	0.00	0.00	N
ATOM	3220	CA	GLY	247	96.020	85.100	65.871	0.00	0.00	C
ATOM	3221	C	GLY	247	95.492	84.695	67.263	0.00	0.00	C
ATOM	3222	O	GLY	247	95.697	85.401	68.254	0.00	0.00	O
ATOM	3223	H	GLY	247	97.934	83.977	65.917	0.00	0.00	H
ATOM	3224	1HA	GLY	247	95.163	85.180	65.173	0.00	0.00	H
ATOM	3225	2HA	GLY	247	96.403	86.132	65.927	0.00	0.00	H
ATOM	3226	N	LYS	248	94.784	83.561	67.320	1.00	0.00	N
ATOM	3227	CA	LYS	248	94.201	83.016	68.579	1.00	0.00	C
ATOM	3228	C	LYS	248	95.191	82.099	69.402	1.00	0.00	C
ATOM	3229	O	LYS	248	95.994	81.382	68.791	1.00	0.00	O
ATOM	3230	CB	LYS	248	92.912	82.231	68.204	1.00	0.00	C
ATOM	3231	CG	LYS	248	91.705	83.103	67.777	1.00	0.00	C
ATOM	3232	CD	LYS	248	90.498	82.257	67.331	1.00	0.00	C
ATOM	3233	CE	LYS	248	89.278	83.127	66.999	1.00	0.00	C
ATOM	3234	NZ	LYS	248	88.159	82.262	66.577	1.00	0.00	N
ATOM	3235	1HZ	LYS	248	87.339	82.845	66.354	1.00	0.00	H
ATOM	3236	2HZ	LYS	248	88.436	81.725	65.743	1.00	0.00	H
ATOM	3237	3HZ	LYS	248	87.920	81.612	67.339	1.00	0.00	H
ATOM	3238	H	LYS	248	94.798	83.034	66.443	1.00	0.00	H
ATOM	3239	HA	LYS	248	93.904	83.868	69.219	1.00	0.00	H
ATOM	3240	1HB	LYS	248	93.145	81.487	67.415	1.00	0.00	H
ATOM	3241	2HB	LYS	248	92.596	81.613	69.067	1.00	0.00	H
ATOM	3242	1HG	LYS	248	91.419	83.774	68.610	1.00	0.00	H
ATOM	3243	2HG	LYS	248	92.002	83.776	66.948	1.00	0.00	H
ATOM	3244	1HD	LYS	248	90.780	81.656	66.443	1.00	0.00	H
ATOM	3245	2HD	LYS	248	90.239	81.516	68.112	1.00	0.00	H
ATOM	3246	1HE	LYS	248	88.979	83.741	67.873	1.00	0.00	H
ATOM	3247	2HE	LYS	248	89.524	83.843	66.188	1.00	0.00	H
ATOM	3248	N	PRO	249	95.154	82.039	70.771	0.00	0.00	N
ATOM	3249	CA	PRO	249	96.020	81.112	71.555	0.00	0.00	C
ATOM	3250	CD	PRO	249	94.324	82.923	71.609	0.00	0.00	C
ATOM	3251	C	PRO	249	95.717	79.571	71.421	0.00	0.00	C
ATOM	3252	O	PRO	249	94.594	79.206	71.051	0.00	0.00	O
ATOM	3253	CB	PRO	249	95.856	81.670	72.986	0.00	0.00	C
ATOM	3254	CG	PRO	249	94.475	82.324	73.005	0.00	0.00	C
ATOM	3255	HA	PRO	249	97.059	81.260	71.214	0.00	0.00	H
ATOM	3256	1HD	PRO	249	93.266	82.947	71.289	0.00	0.00	H
ATOM	3257	2HD	PRO	249	94.709	83.962	71.575	0.00	0.00	H
ATOM	3258	1HB	PRO	249	96.635	82.431	73.179	0.00	0.00	H
ATOM	3259	2HB	PRO	249	95.969	80.898	73.772	0.00	0.00	H
ATOM	3260	1HG	PRO	249	94.358	83.079	73.801	0.00	0.00	H
ATOM	3261	2HG	PRO	249	93.697	81.554	73.164	0.00	0.00	H
ATOM	3262	N	PRO	250	96.669	78.630	71.710	0.00	0.00	N

ATOM	3263	CA	PRO	250	96.501	77.190	71.345	0.00	0.00	C
ATOM	3264	CD	PRO	250	98.027	78.957	72.199	0.00	0.00	C
ATOM	3265	C	PRO	250	95.405	76.338	72.063	0.00	0.00	C
ATOM	3266	O	PRO	250	94.769	75.510	71.408	0.00	0.00	O
ATOM	3267	CB	PRO	250	97.937	76.661	71.500	0.00	0.00	C
ATOM	3268	CG	PRO	250	98.615	77.582	72.511	0.00	0.00	C
ATOM	3269	HA	PRO	250	96.236	77.132	70.273	0.00	0.00	H
ATOM	3270	1HD	PRO	250	98.022	79.609	73.093	0.00	0.00	H
ATOM	3271	2HD	PRO	250	98.612	79.473	71.412	0.00	0.00	H
ATOM	3272	1HB	PRO	250	98.465	76.713	70.531	0.00	0.00	H
ATOM	3273	2HB	PRO	250	97.983	75.602	71.782	0.00	0.00	H
ATOM	3274	1HG	PRO	250	99.717	77.552	72.427	0.00	0.00	H
ATOM	3275	2HG	PRO	250	98.359	77.276	73.544	0.00	0.00	H
ATOM	3276	N	PHE	251	95.171	76.536	73.369	0.00	0.00	N
ATOM	3277	CA	PHE	251	93.963	75.999	74.056	0.00	0.00	C
ATOM	3278	C	PHE	251	93.134	77.170	74.676	0.00	0.00	C
ATOM	3279	O	PHE	251	93.535	77.784	75.669	0.00	0.00	O
ATOM	3280	CB	PHE	251	94.359	74.924	75.110	0.00	0.00	C
ATOM	3281	CG	PHE	251	94.855	73.539	74.627	0.00	0.00	C
ATOM	3282	CD1	PHE	251	94.370	72.914	73.468	0.00	0.00	C
ATOM	3283	CE1	PHE	251	94.778	71.624	73.136	0.00	0.00	C
ATOM	3284	CZ	PHE	251	95.658	70.940	73.966	0.00	0.00	C
ATOM	3285	CE2	PHE	251	96.139	71.542	75.122	0.00	0.00	C
ATOM	3286	CD2	PHE	251	95.739	72.836	75.452	0.00	0.00	C
ATOM	3287	H	PHE	251	95.711	77.322	73.743	0.00	0.00	H
ATOM	3288	HA	PHE	251	93.295	75.495	73.329	0.00	0.00	H
ATOM	3289	1HB	PHE	251	93.478	74.727	75.750	0.00	0.00	H
ATOM	3290	2HB	PHE	251	95.092	75.375	75.806	0.00	0.00	H
ATOM	3291	HD1	PHE	251	93.671	73.410	72.814	0.00	0.00	H
ATOM	3292	HE1	PHE	251	94.410	71.151	72.236	0.00	0.00	H
ATOM	3293	HZ	PHE	251	95.972	69.941	73.707	0.00	0.00	H
ATOM	3294	HE2	PHE	251	96.825	71.005	75.763	0.00	0.00	H
ATOM	3295	HD2	PHE	251	96.115	73.283	76.358	0.00	0.00	H
ATOM	3296	N	GLU	252	91.963	77.457	74.083	1.00	0.00	N
ATOM	3297	CA	GLU	252	90.978	78.433	74.629	1.00	0.00	C
ATOM	3298	C	GLU	252	89.511	77.887	74.512	1.00	0.00	C
ATOM	3299	O	GLU	252	88.774	78.205	73.573	1.00	0.00	O
ATOM	3300	CB	GLU	252	91.191	79.843	74.006	1.00	0.00	C
ATOM	3301	CG	GLU	252	91.120	79.990	72.457	1.00	0.00	C
ATOM	3302	CD	GLU	252	90.880	81.410	71.943	1.00	0.00	C
ATOM	3303	OE1	GLU	252	91.116	82.435	72.575	1.00	0.00	O
ATOM	3304	OE2	GLU	252	90.369	81.410	70.683	1.00	0.00	O
ATOM	3305	H	GLU	252	91.798	76.958	73.202	1.00	0.00	H
ATOM	3306	HA	GLU	252	91.157	78.567	75.716	1.00	0.00	H
ATOM	3307	1HB	GLU	252	90.450	80.523	74.472	1.00	0.00	H
ATOM	3308	2HB	GLU	252	92.170	80.226	74.346	1.00	0.00	H
ATOM	3309	1HG	GLU	252	92.052	79.611	71.998	1.00	0.00	H
ATOM	3310	2HG	GLU	252	90.319	79.351	72.044	1.00	0.00	H
ATOM	3311	N	THR	253	89.078	77.064	75.479	1.00	0.00	N
ATOM	3312	CA	THR	253	87.671	76.555	75.551	1.00	0.00	C
ATOM	3313	C	THR	253	86.821	77.456	76.525	1.00	0.00	C
ATOM	3314	O	THR	253	87.348	78.092	77.442	1.00	0.00	O
ATOM	3315	CB	THR	253	87.705	75.025	75.879	1.00	0.00	C
ATOM	3316	OG1	THR	253	88.536	74.338	74.942	1.00	0.00	O
ATOM	3317	CG2	THR	253	86.347	74.314	75.773	1.00	0.00	C
ATOM	3318	H	THR	253	89.751	76.885	76.233	1.00	0.00	H
ATOM	3319	HA	THR	253	87.207	76.633	74.548	1.00	0.00	H
ATOM	3320	HB	THR	253	88.122	74.883	76.897	1.00	0.00	H
ATOM	3321	HG1	THR	253	88.566	73.395	75.177	1.00	0.00	H
ATOM	3322	1HG2	THR	253	86.442	73.235	76.002	1.00	0.00	H
ATOM	3323	2HG2	THR	253	85.601	74.722	76.478	1.00	0.00	H
ATOM	3324	3HG2	THR	253	85.921	74.392	74.756	1.00	0.00	H
ATOM	3325	N	SER	254	85.496	77.557	76.310	1.00	0.00	N
ATOM	3326	CA	SER	254	84.656	78.676	76.858	1.00	0.00	C
ATOM	3327	C	SER	254	84.494	78.929	78.410	1.00	0.00	C
ATOM	3328	O	SER	254	83.812	79.888	78.786	1.00	0.00	O
ATOM	3329	CB	SER	254	83.275	78.531	76.169	1.00	0.00	C
ATOM	3330	OG	SER	254	82.460	79.682	76.403	1.00	0.00	O
ATOM	3331	H	SER	254	85.181	77.003	75.509	1.00	0.00	H
ATOM	3332	HA	SER	254	85.095	79.620	76.478	1.00	0.00	H
ATOM	3333	1HB	SER	254	83.378	78.402	75.073	1.00	0.00	H
ATOM	3334	2HB	SER	254	82.749	77.626	76.532	1.00	0.00	H
ATOM	3335	HG	SER	254	82.592	79.944	77.326	1.00	0.00	H

ATOM	3336	N	CYS	255	85.100	78.129	79.298	1.00	0.00	N
ATOM	3337	CA	CYS	255	85.274	78.483	80.735	1.00	0.00	C
ATOM	3338	C	CYS	255	86.653	77.980	81.291	1.00	0.00	C
ATOM	3339	O	CYS	255	87.287	77.081	80.727	1.00	0.00	O
ATOM	3340	CB	CYS	255	84.059	77.949	81.532	1.00	0.00	C
ATOM	3341	SG	CYS	255	83.991	76.125	81.530	1.00	0.00	S
ATOM	3342	H	CYS	255	85.801	77.541	78.829	1.00	0.00	H
ATOM	3343	HA	CYS	255	85.285	79.588	80.834	1.00	0.00	H
ATOM	3344	1HB	CYS	255	84.098	78.298	82.579	1.00	0.00	H
ATOM	3345	2HB	CYS	255	83.111	78.350	81.122	1.00	0.00	H
ATOM	3346	HG	CYS	255	83.576	75.982	80.275	1.00	0.00	H
ATOM	3347	N	LEU	256	87.110	78.539	82.429	1.00	0.00	N
ATOM	3348	CA	LEU	256	88.437	78.204	83.043	1.00	0.00	C
ATOM	3349	C	LEU	256	88.717	76.678	83.289	1.00	0.00	C
ATOM	3350	O	LEU	256	89.732	76.166	82.819	1.00	0.00	O
ATOM	3351	CB	LEU	256	88.641	79.036	84.347	1.00	0.00	C
ATOM	3352	CG	LEU	256	88.951	80.551	84.214	1.00	0.00	C
ATOM	3353	CD1	LEU	256	87.723	81.413	83.867	1.00	0.00	C
ATOM	3354	CD2	LEU	256	89.546	81.077	85.533	1.00	0.00	C
ATOM	3355	H	LEU	256	86.525	79.294	82.798	1.00	0.00	H
ATOM	3356	HA	LEU	256	89.222	78.522	82.328	1.00	0.00	H
ATOM	3357	1HB	LEU	256	87.794	78.878	85.043	1.00	0.00	H
ATOM	3358	2HB	LEU	256	89.502	78.580	84.880	1.00	0.00	H
ATOM	3359	HG	LEU	256	89.710	80.687	83.419	1.00	0.00	H
ATOM	3360	2HD1	LEU	256	87.335	81.198	82.857	1.00	0.00	H
ATOM	3361	3HD1	LEU	256	86.893	81.266	84.584	1.00	0.00	H
ATOM	3362	1HD1	LEU	256	87.965	82.492	83.872	1.00	0.00	H
ATOM	3363	2HD2	LEU	256	88.839	80.978	86.380	1.00	0.00	H
ATOM	3364	3HD2	LEU	256	90.465	80.530	85.818	1.00	0.00	H
ATOM	3365	1HD2	LEU	256	89.825	82.144	85.467	1.00	0.00	H
ATOM	3366	N	LYS	257	87.800	75.951	83.953	1.00	0.00	N
ATOM	3367	CA	LYS	257	87.873	74.462	84.089	1.00	0.00	C
ATOM	3368	C	LYS	257	87.861	73.614	82.764	1.00	0.00	C
ATOM	3369	O	LYS	257	88.490	72.555	82.727	1.00	0.00	O
ATOM	3370	CB	LYS	257	86.754	74.003	85.066	1.00	0.00	C
ATOM	3371	CG	LYS	257	86.922	74.460	86.537	1.00	0.00	C
ATOM	3372	CD	LYS	257	85.765	73.981	87.434	1.00	0.00	C
ATOM	3373	CE	LYS	257	85.926	74.466	88.881	1.00	0.00	C
ATOM	3374	NZ	LYS	257	84.781	73.996	89.685	1.00	0.00	N
ATOM	3375	1HZ	LYS	257	84.887	74.321	90.657	1.00	0.00	H
ATOM	3376	2HZ	LYS	257	83.906	74.372	89.292	1.00	0.00	H
ATOM	3377	3HZ	LYS	257	84.749	72.967	89.670	1.00	0.00	H
ATOM	3378	H	LYS	257	86.991	76.492	84.272	1.00	0.00	H
ATOM	3379	HA	LYS	257	88.840	74.217	84.568	1.00	0.00	H
ATOM	3380	1HB	LYS	257	85.766	74.319	84.678	1.00	0.00	H
ATOM	3381	2HB	LYS	257	86.711	72.897	85.064	1.00	0.00	H
ATOM	3382	1HG	LYS	257	87.885	74.087	86.937	1.00	0.00	H
ATOM	3383	2HG	LYS	257	86.992	75.564	86.588	1.00	0.00	H
ATOM	3384	1HD	LYS	257	84.800	74.343	87.025	1.00	0.00	H
ATOM	3385	2HD	LYS	257	85.706	72.875	87.407	1.00	0.00	H
ATOM	3386	1HE	LYS	257	86.877	74.097	89.316	1.00	0.00	H
ATOM	3387	2HE	LYS	257	85.978	75.573	88.918	1.00	0.00	H
ATOM	3388	N	GLU	258	87.189	74.064	81.686	1.00	0.00	N
ATOM	3389	CA	GLU	258	87.332	73.448	80.332	1.00	0.00	C
ATOM	3390	C	GLU	258	88.705	73.711	79.619	1.00	0.00	C
ATOM	3391	O	GLU	258	89.293	72.754	79.114	1.00	0.00	O
ATOM	3392	CB	GLU	258	86.118	73.847	79.451	1.00	0.00	C
ATOM	3393	CG	GLU	258	84.750	73.213	79.823	1.00	0.00	C
ATOM	3394	CD	GLU	258	84.645	71.709	79.571	1.00	0.00	C
ATOM	3395	OE1	GLU	258	84.362	71.217	78.485	1.00	0.00	O
ATOM	3396	OE2	GLU	258	84.899	70.977	80.687	1.00	0.00	O
ATOM	3397	H	GLU	258	86.861	75.028	81.801	1.00	0.00	H
ATOM	3398	HA	GLU	258	87.289	72.346	80.451	1.00	0.00	H
ATOM	3399	1HB	GLU	258	86.027	74.951	79.425	1.00	0.00	H
ATOM	3400	2HB	GLU	258	86.339	73.566	78.406	1.00	0.00	H
ATOM	3401	1HG	GLU	258	84.495	73.423	80.877	1.00	0.00	H
ATOM	3402	2HG	GLU	258	83.951	73.695	79.230	1.00	0.00	H
ATOM	3403	N	THR	259	89.256	74.941	79.608	1.00	0.00	N
ATOM	3404	CA	THR	259	90.700	75.186	79.255	1.00	0.00	C
ATOM	3405	C	THR	259	91.743	74.348	80.089	1.00	0.00	C
ATOM	3406	O	THR	259	92.662	73.765	79.509	1.00	0.00	O
ATOM	3407	CB	THR	259	90.988	76.720	79.303	1.00	0.00	C
ATOM	3408	OG1	THR	259	90.192	77.414	78.352	1.00	0.00	O

ATOM	3409	CG2	THR	259	92.425	77.133	78.955	1.00	0.00	C
ATOM	3410	H	THR	259	88.665	75.681	80.011	1.00	0.00	H
ATOM	3411	HA	THR	259	90.841	74.870	78.203	1.00	0.00	H
ATOM	3412	HB	THR	259	90.750	77.097	80.320	1.00	0.00	H
ATOM	3413	HG1	THR	259	90.577	78.292	78.280	1.00	0.00	H
ATOM	3414	1HG2	THR	259	92.562	78.226	79.020	1.00	0.00	H
ATOM	3415	2HG2	THR	259	93.166	76.690	79.646	1.00	0.00	H
ATOM	3416	3HG2	THR	259	92.711	76.823	77.933	1.00	0.00	H
ATOM	3417	N	TYR	260	91.586	74.262	81.423	0.00	0.00	N
ATOM	3418	CA	TYR	260	92.363	73.330	82.294	0.00	0.00	C
ATOM	3419	C	TYR	260	92.279	71.804	81.919	0.00	0.00	C
ATOM	3420	O	TYR	260	93.315	71.139	81.844	0.00	0.00	O
ATOM	3421	CB	TYR	260	91.924	73.570	83.770	0.00	0.00	C
ATOM	3422	CG	TYR	260	92.128	74.943	84.457	0.00	0.00	C
ATOM	3423	CD1	TYR	260	92.987	75.934	83.963	0.00	0.00	C
ATOM	3424	CE1	TYR	260	93.105	77.157	84.618	0.00	0.00	C
ATOM	3425	CZ	TYR	260	92.370	77.402	85.772	0.00	0.00	C
ATOM	3426	OH	TYR	260	92.494	78.601	86.417	0.00	0.00	O
ATOM	3427	CE2	TYR	260	91.523	76.424	86.280	0.00	0.00	C
ATOM	3428	CD2	TYR	260	91.408	75.196	85.631	0.00	0.00	C
ATOM	3429	H	TYR	260	90.890	74.876	81.869	1.00	0.00	H
ATOM	3430	HA	TYR	260	93.435	73.594	82.207	0.00	0.00	H
ATOM	3431	1HB	TYR	260	92.431	72.818	84.399	0.00	0.00	H
ATOM	3432	2HB	TYR	260	90.856	73.289	83.848	0.00	0.00	H
ATOM	3433	HD1	TYR	260	93.564	75.768	83.063	0.00	0.00	H
ATOM	3434	HE1	TYR	260	93.777	77.903	84.231	0.00	0.00	H
ATOM	3435	HH	TYR	260	93.285	79.038	86.094	0.00	0.00	H
ATOM	3436	HE2	TYR	260	90.964	76.616	87.184	0.00	0.00	H
ATOM	3437	HD2	TYR	260	90.752	74.444	86.046	0.00	0.00	H
ATOM	3438	N	LEU	261	91.075	71.265	81.640	1.00	0.00	N
ATOM	3439	CA	LEU	261	90.897	69.932	80.984	1.00	0.00	C
ATOM	3440	C	LEU	261	91.694	69.702	79.646	1.00	0.00	C
ATOM	3441	O	LEU	261	92.322	68.652	79.497	1.00	0.00	O
ATOM	3442	CB	LEU	261	89.358	69.723	80.849	1.00	0.00	C
ATOM	3443	CG	LEU	261	88.856	68.354	80.325	1.00	0.00	C
ATOM	3444	CD1	LEU	261	89.165	67.203	81.298	1.00	0.00	C
ATOM	3445	CD2	LEU	261	87.340	68.412	80.075	1.00	0.00	C
ATOM	3446	H	LEU	261	90.292	71.922	81.746	1.00	0.00	H
ATOM	3447	HA	LEU	261	91.277	69.171	81.692	1.00	0.00	H
ATOM	3448	1HB	LEU	261	88.869	69.924	81.824	1.00	0.00	H
ATOM	3449	2HB	LEU	261	88.967	70.510	80.178	1.00	0.00	H
ATOM	3450	HG	LEU	261	89.350	68.138	79.355	1.00	0.00	H
ATOM	3451	2HD1	LEU	261	90.254	67.069	81.437	1.00	0.00	H
ATOM	3452	3HD1	LEU	261	88.721	67.367	82.298	1.00	0.00	H
ATOM	3453	1HD1	LEU	261	88.781	66.236	80.922	1.00	0.00	H
ATOM	3454	2HD2	LEU	261	86.774	68.623	81.001	1.00	0.00	H
ATOM	3455	3HD2	LEU	261	87.082	69.198	79.340	1.00	0.00	H
ATOM	3456	1HD2	LEU	261	86.959	67.459	79.664	1.00	0.00	H
ATOM	3457	N	ARG	262	91.731	70.679	78.720	1.00	0.00	N
ATOM	3458	CA	ARG	262	92.648	70.647	77.542	1.00	0.00	C
ATOM	3459	C	ARG	262	94.188	70.612	77.880	1.00	0.00	C
ATOM	3460	O	ARG	262	94.905	69.763	77.348	1.00	0.00	O
ATOM	3461	CB	ARG	262	92.340	71.831	76.577	1.00	0.00	C
ATOM	3462	CG	ARG	262	90.899	72.128	76.094	1.00	0.00	C
ATOM	3463	CD	ARG	262	90.194	70.966	75.385	1.00	0.00	C
ATOM	3464	NE	ARG	262	88.899	71.458	74.845	1.00	0.00	N
ATOM	3465	CZ	ARG	262	88.061	70.748	74.099	1.00	0.00	C
ATOM	3466	NH1	ARG	262	88.245	69.501	73.778	1.00	0.00	N
ATOM	3467	NH2	ARG	262	87.005	71.337	73.662	1.00	0.00	N
ATOM	3468	HE	ARG	262	88.631	72.428	75.067	1.00	0.00	H
ATOM	3469	H	ARG	262	91.155	71.497	78.953	1.00	0.00	H
ATOM	3470	HA	ARG	262	92.440	69.712	76.984	1.00	0.00	H
ATOM	3471	1HB	ARG	262	92.731	72.763	77.029	1.00	0.00	H
ATOM	3472	2HB	ARG	262	92.961	71.684	75.673	1.00	0.00	H
ATOM	3473	1HG	ARG	262	90.280	72.468	76.943	1.00	0.00	H
ATOM	3474	2HG	ARG	262	90.939	73.002	75.413	1.00	0.00	H
ATOM	3475	1HD	ARG	262	90.835	70.574	74.570	1.00	0.00	H
ATOM	3476	2HD	ARG	262	90.030	70.128	76.095	1.00	0.00	H
ATOM	3477	2HH1	ARG	262	89.103	69.110	74.168	1.00	0.00	H
ATOM	3478	1HH1	ARG	262	87.536	69.062	73.194	1.00	0.00	H
ATOM	3479	1HH2	ARG	262	86.968	72.323	73.921	1.00	0.00	H
ATOM	3480	2HH2	ARG	262	86.383	70.796	73.065	1.00	0.00	H
ATOM	3481	N	ILE	263	94.699	71.521	78.739	0.00	0.00	N

ATOM	3482	CA	ILE	263	96.162	71.638	79.087	0.00	0.00	C
ATOM	3483	C	ILE	263	96.852	70.322	79.595	0.00	0.00	C
ATOM	3484	O	ILE	263	97.919	69.961	79.089	0.00	0.00	O
ATOM	3485	CB	ILE	263	96.358	72.915	79.998	0.00	0.00	C
ATOM	3486	CG2	ILE	263	97.713	72.981	80.760	0.00	0.00	C
ATOM	3487	CG1	ILE	263	96.180	74.229	79.176	0.00	0.00	C
ATOM	3488	CD1	ILE	263	96.033	75.524	79.988	0.00	0.00	C
ATOM	3489	H	ILE	263	93.987	72.147	79.138	0.00	0.00	H
ATOM	3490	HA	ILE	263	96.703	71.848	78.143	0.00	0.00	H
ATOM	3491	HB	ILE	263	95.570	72.886	80.779	0.00	0.00	H
ATOM	3492	1HG2	ILE	263	97.758	73.841	81.453	0.00	0.00	H
ATOM	3493	2HG2	ILE	263	97.888	72.090	81.391	0.00	0.00	H
ATOM	3494	3HG2	ILE	263	98.576	73.073	80.078	0.00	0.00	H
ATOM	3495	1HG1	ILE	263	95.276	74.150	78.541	0.00	0.00	H
ATOM	3496	2HG1	ILE	263	97.018	74.342	78.460	0.00	0.00	H
ATOM	3497	1HD1	ILE	263	95.825	76.385	79.327	0.00	0.00	H
ATOM	3498	2HD1	ILE	263	95.201	75.466	80.716	0.00	0.00	H
ATOM	3499	3HD1	ILE	263	96.952	75.777	80.549	0.00	0.00	H
ATOM	3500	N	LYS	264	96.248	69.602	80.554	1.00	0.00	N
ATOM	3501	CA	LYS	264	96.726	68.247	80.970	1.00	0.00	C
ATOM	3502	C	LYS	264	96.706	67.106	79.876	1.00	0.00	C
ATOM	3503	O	LYS	264	97.548	66.207	79.928	1.00	0.00	O
ATOM	3504	CB	LYS	264	95.936	67.915	82.266	1.00	0.00	C
ATOM	3505	CG	LYS	264	96.507	66.746	83.102	1.00	0.00	C
ATOM	3506	CD	LYS	264	95.859	66.668	84.497	1.00	0.00	C
ATOM	3507	CE	LYS	264	96.455	65.540	85.352	1.00	0.00	C
ATOM	3508	NZ	LYS	264	95.990	65.686	86.747	1.00	0.00	N
ATOM	3509	1HZ	LYS	264	96.389	64.930	87.323	1.00	0.00	H
ATOM	3510	2HZ	LYS	264	96.296	66.597	87.118	1.00	0.00	H
ATOM	3511	3HZ	LYS	264	94.962	65.631	86.775	1.00	0.00	H
ATOM	3512	H	LYS	264	95.332	69.978	80.830	1.00	0.00	H
ATOM	3513	HA	LYS	264	97.791	68.352	81.256	1.00	0.00	H
ATOM	3514	1HB	LYS	264	95.915	68.811	82.921	1.00	0.00	H
ATOM	3515	2HB	LYS	264	94.873	67.717	82.021	1.00	0.00	H
ATOM	3516	1HG	LYS	264	96.375	65.790	82.559	1.00	0.00	H
ATOM	3517	2HG	LYS	264	97.603	66.872	83.218	1.00	0.00	H
ATOM	3518	1HD	LYS	264	95.990	67.646	85.005	1.00	0.00	H
ATOM	3519	2HD	LYS	264	94.763	66.533	84.400	1.00	0.00	H
ATOM	3520	1HE	LYS	264	96.164	64.551	84.944	1.00	0.00	H
ATOM	3521	2HE	LYS	264	97.564	65.563	85.324	1.00	0.00	H
ATOM	3522	N	LYS	265	95.801	67.156	78.879	1.00	0.00	N
ATOM	3523	CA	LYS	265	95.810	66.235	77.699	1.00	0.00	C
ATOM	3524	C	LYS	265	96.949	66.440	76.629	1.00	0.00	C
ATOM	3525	O	LYS	265	97.292	65.473	75.946	1.00	0.00	O
ATOM	3526	CB	LYS	265	94.419	66.320	77.003	1.00	0.00	C
ATOM	3527	CG	LYS	265	93.209	65.795	77.809	1.00	0.00	C
ATOM	3528	CD	LYS	265	91.881	66.006	77.056	1.00	0.00	C
ATOM	3529	CE	LYS	265	90.672	65.560	77.889	1.00	0.00	C
ATOM	3530	NZ	LYS	265	89.430	65.791	77.125	1.00	0.00	N
ATOM	3531	1HZ	LYS	265	88.620	65.492	77.686	1.00	0.00	H
ATOM	3532	2HZ	LYS	265	89.343	66.794	76.905	1.00	0.00	H
ATOM	3533	3HZ	LYS	265	89.460	65.250	76.249	1.00	0.00	H
ATOM	3534	H	LYS	265	95.178	67.973	78.921	1.00	0.00	H
ATOM	3535	HA	LYS	265	95.937	65.197	78.066	1.00	0.00	H
ATOM	3536	1HB	LYS	265	94.232	67.367	76.691	1.00	0.00	H
ATOM	3537	2HB	LYS	265	94.456	65.750	76.053	1.00	0.00	H
ATOM	3538	1HG	LYS	265	93.348	64.723	78.049	1.00	0.00	H
ATOM	3539	2HG	LYS	265	93.160	66.311	78.789	1.00	0.00	H
ATOM	3540	1HD	LYS	265	91.772	67.079	76.801	1.00	0.00	H
ATOM	3541	2HD	LYS	265	91.908	65.464	76.090	1.00	0.00	H
ATOM	3542	1HE	LYS	265	90.760	64.492	78.170	1.00	0.00	H
ATOM	3543	2HE	LYS	265	90.640	66.128	78.842	1.00	0.00	H
ATOM	3544	N	ASN	266	97.497	67.659	76.420	1.00	0.00	N
ATOM	3545	CA	ASN	266	98.622	67.927	75.454	1.00	0.00	C
ATOM	3546	C	ASN	266	98.354	67.785	73.900	1.00	0.00	C
ATOM	3547	O	ASN	266	99.262	68.052	73.108	1.00	0.00	O
ATOM	3548	CB	ASN	266	99.918	67.198	75.952	1.00	0.00	C
ATOM	3549	CG	ASN	266	101.331	67.657	75.554	1.00	0.00	C
ATOM	3550	OD1	ASN	266	102.317	67.035	75.926	1.00	0.00	O
ATOM	3551	ND2	ASN	266	101.533	68.726	74.836	1.00	0.00	N
ATOM	3552	H	ASN	266	97.146	68.365	77.079	1.00	0.00	H
ATOM	3553	HA	ASN	266	98.819	69.010	75.570	1.00	0.00	H
ATOM	3554	1HB	ASN	266	99.928	67.201	77.057	1.00	0.00	H

ATOM	3555	2HB	ASN	266	99.845	66.127	75.691	1.00	0.00	H
ATOM	3556	1HD2	ASN	266	102.525	68.892	74.616	1.00	0.00	H
ATOM	3557	2HD2	ASN	266	100.737	68.989	74.248	1.00	0.00	H
ATOM	3558	N	GLU	267	97.150	67.411	73.431	1.00	0.00	N
ATOM	3559	CA	GLU	267	96.876	67.153	71.985	1.00	0.00	C
ATOM	3560	C	GLU	267	96.696	68.462	71.129	1.00	0.00	C
ATOM	3561	O	GLU	267	95.588	68.985	70.971	1.00	0.00	O
ATOM	3562	CB	GLU	267	95.662	66.183	71.946	1.00	0.00	C
ATOM	3563	CG	GLU	267	95.357	65.583	70.549	1.00	0.00	C
ATOM	3564	CD	GLU	267	94.191	64.600	70.541	1.00	0.00	C
ATOM	3565	OE1	GLU	267	94.308	63.397	70.740	1.00	0.00	O
ATOM	3566	OE2	GLU	267	93.002	65.207	70.284	1.00	0.00	O
ATOM	3567	H	GLU	267	96.511	67.122	74.178	1.00	0.00	H
ATOM	3568	HA	GLU	267	97.734	66.589	71.560	1.00	0.00	H
ATOM	3569	1HB	GLU	267	95.833	65.341	72.650	1.00	0.00	H
ATOM	3570	2HB	GLU	267	94.761	66.704	72.329	1.00	0.00	H
ATOM	3571	1HG	GLU	267	95.145	66.387	69.818	1.00	0.00	H
ATOM	3572	2HG	GLU	267	96.246	65.055	70.155	1.00	0.00	H
ATOM	3573	N	TYR	268	97.801	68.977	70.566	1.00	0.00	N
ATOM	3574	CA	TYR	268	97.809	70.263	69.810	1.00	0.00	C
ATOM	3575	C	TYR	268	97.716	70.049	68.260	1.00	0.00	C
ATOM	3576	O	TYR	268	98.681	69.627	67.613	1.00	0.00	O
ATOM	3577	CB	TYR	268	99.087	71.069	70.197	1.00	0.00	C
ATOM	3578	CG	TYR	268	99.105	71.681	71.610	1.00	0.00	C
ATOM	3579	CD1	TYR	268	99.934	71.160	72.610	1.00	0.00	C
ATOM	3580	CD2	TYR	268	98.293	72.781	71.901	1.00	0.00	C
ATOM	3581	CE1	TYR	268	99.936	71.723	73.886	1.00	0.00	C
ATOM	3582	CE2	TYR	268	98.311	73.348	73.172	1.00	0.00	C
ATOM	3583	CZ	TYR	268	99.135	72.824	74.159	1.00	0.00	C
ATOM	3584	OH	TYR	268	99.129	73.384	75.404	1.00	0.00	O
ATOM	3585	H	TYR	268	98.686	68.459	70.662	1.00	0.00	H
ATOM	3586	HA	TYR	268	96.943	70.887	70.118	1.00	0.00	H
ATOM	3587	1HB	TYR	268	99.988	70.447	70.028	1.00	0.00	H
ATOM	3588	2HB	TYR	268	99.218	71.902	69.480	1.00	0.00	H
ATOM	3589	HD1	TYR	268	100.574	70.315	72.401	1.00	0.00	H
ATOM	3590	HD2	TYR	268	97.630	73.189	71.151	1.00	0.00	H
ATOM	3591	HE1	TYR	268	100.564	71.324	74.667	1.00	0.00	H
ATOM	3592	HE2	TYR	268	97.647	74.166	73.408	1.00	0.00	H
ATOM	3593	HH	TYR	268	98.543	74.141	75.387	1.00	0.00	H
ATOM	3594	N	SER	269	96.568	70.395	67.653	1.00	0.00	N
ATOM	3595	CA	SER	269	96.405	70.397	66.171	1.00	0.00	C
ATOM	3596	C	SER	269	96.971	71.702	65.513	1.00	0.00	C
ATOM	3597	O	SER	269	96.390	72.782	65.646	1.00	0.00	O
ATOM	3598	CB	SER	269	94.904	70.187	65.869	1.00	0.00	C
ATOM	3599	OG	SER	269	94.671	70.101	64.462	1.00	0.00	O
ATOM	3600	H	SER	269	95.820	70.687	68.289	1.00	0.00	H
ATOM	3601	HA	SER	269	96.930	69.519	65.741	1.00	0.00	H
ATOM	3602	1HB	SER	269	94.538	69.257	66.349	1.00	0.00	H
ATOM	3603	2HB	SER	269	94.294	71.008	66.298	1.00	0.00	H
ATOM	3604	HG	SER	269	94.931	70.946	64.075	1.00	0.00	H
ATOM	3605	N	ILE	270	98.101	71.600	64.796	1.00	0.00	N
ATOM	3606	CA	ILE	270	98.790	72.785	64.192	1.00	0.00	C
ATOM	3607	C	ILE	270	98.061	73.392	62.921	1.00	0.00	C
ATOM	3608	O	ILE	270	97.670	72.619	62.038	1.00	0.00	O
ATOM	3609	CB	ILE	270	100.313	72.516	63.902	1.00	0.00	C
ATOM	3610	CG1	ILE	270	100.607	71.347	62.913	1.00	0.00	C
ATOM	3611	CG2	ILE	270	101.142	72.357	65.205	1.00	0.00	C
ATOM	3612	CD1	ILE	270	101.972	71.429	62.207	1.00	0.00	C
ATOM	3613	H	ILE	270	98.550	70.680	64.833	1.00	0.00	H
ATOM	3614	HA	ILE	270	98.791	73.563	64.976	1.00	0.00	H
ATOM	3615	HB	ILE	270	100.692	73.441	63.419	1.00	0.00	H
ATOM	3616	1HG1	ILE	270	100.504	70.372	63.427	1.00	0.00	H
ATOM	3617	2HG1	ILE	270	99.834	71.324	62.120	1.00	0.00	H
ATOM	3618	2HG2	ILE	270	101.005	73.213	65.890	1.00	0.00	H
ATOM	3619	3HG2	ILE	270	100.862	71.445	65.766	1.00	0.00	H
ATOM	3620	1HG2	ILE	270	102.227	72.289	65.001	1.00	0.00	H
ATOM	3621	2HD1	ILE	270	102.088	72.375	61.642	1.00	0.00	H
ATOM	3622	3HD1	ILE	270	102.809	71.363	62.922	1.00	0.00	H
ATOM	3623	1HD1	ILE	270	102.101	70.606	61.481	1.00	0.00	H
ATOM	3624	N	PRO	271	97.905	74.741	62.737	0.00	0.00	N
ATOM	3625	CA	PRO	271	97.452	75.329	61.445	0.00	0.00	C
ATOM	3626	CD	PRO	271	98.045	75.733	63.816	0.00	0.00	C
ATOM	3627	C	PRO	271	98.411	75.108	60.225	0.00	0.00	C

ATOM	3628	O	PRO	271	99.637	75.076	60.365	0.00	0.00	O
ATOM	3629	CB	PRO	271	97.285	76.826	61.795	0.00	0.00	C
ATOM	3630	CG	PRO	271	97.187	76.890	63.320	0.00	0.00	C
ATOM	3631	HA	PRO	271	96.457	74.900	61.214	0.00	0.00	H
ATOM	3632	1HD	PRO	271	99.104	76.028	63.948	0.00	0.00	H
ATOM	3633	2HD	PRO	271	97.663	75.374	64.789	0.00	0.00	H
ATOM	3634	1HB	PRO	271	96.401	77.273	61.302	0.00	0.00	H
ATOM	3635	2HB	PRO	271	98.155	77.425	61.460	0.00	0.00	H
ATOM	3636	1HG	PRO	271	96.138	76.747	63.647	0.00	0.00	H
ATOM	3637	2HG	PRO	271	97.527	77.855	63.736	0.00	0.00	H
ATOM	3638	N	LYS	272	97.848	75.012	59.012	1.00	0.00	N
ATOM	3639	CA	LYS	272	98.620	74.638	57.781	1.00	0.00	C
ATOM	3640	C	LYS	272	99.753	75.604	57.258	1.00	0.00	C
ATOM	3641	O	LYS	272	100.562	75.181	56.429	1.00	0.00	O
ATOM	3642	CB	LYS	272	97.590	74.311	56.660	1.00	0.00	C
ATOM	3643	CG	LYS	272	96.728	73.042	56.890	1.00	0.00	C
ATOM	3644	CD	LYS	272	95.734	72.788	55.741	1.00	0.00	C
ATOM	3645	CE	LYS	272	94.875	71.542	55.996	1.00	0.00	C
ATOM	3646	NZ	LYS	272	93.936	71.353	54.873	1.00	0.00	N
ATOM	3647	1HZ	LYS	272	93.359	70.516	55.044	1.00	0.00	H
ATOM	3648	2HZ	LYS	272	93.326	72.179	54.792	1.00	0.00	H
ATOM	3649	3HZ	LYS	272	94.465	71.231	53.998	1.00	0.00	H
ATOM	3650	H	LYS	272	96.826	74.945	59.037	1.00	0.00	H
ATOM	3651	HA	LYS	272	99.166	73.697	58.001	1.00	0.00	H
ATOM	3652	1HB	LYS	272	96.940	75.189	56.482	1.00	0.00	H
ATOM	3653	2HB	LYS	272	98.135	74.172	55.706	1.00	0.00	H
ATOM	3654	1HG	LYS	272	97.390	72.162	57.013	1.00	0.00	H
ATOM	3655	2HG	LYS	272	96.173	73.124	57.844	1.00	0.00	H
ATOM	3656	1HD	LYS	272	95.079	73.673	55.612	1.00	0.00	H
ATOM	3657	2HD	LYS	272	96.288	72.683	54.786	1.00	0.00	H
ATOM	3658	1HE	LYS	272	95.515	70.644	56.117	1.00	0.00	H
ATOM	3659	2HE	LYS	272	94.310	71.646	56.944	1.00	0.00	H
ATOM	3660	N	HIS	273	99.852	76.859	57.732	0.00	0.00	N
ATOM	3661	CA	HIS	273	101.068	77.716	57.532	0.00	0.00	C
ATOM	3662	C	HIS	273	102.303	77.505	58.495	0.00	0.00	C
ATOM	3663	O	HIS	273	103.356	78.106	58.261	0.00	0.00	O
ATOM	3664	CB	HIS	273	100.609	79.199	57.426	0.00	0.00	C
ATOM	3665	CG	HIS	273	100.004	79.854	58.670	0.00	0.00	C
ATOM	3666	ND1	HIS	273	100.759	80.491	59.641	0.00	0.00	N
ATOM	3667	CE1	HIS	273	99.745	80.966	60.435	0.00	0.00	C
ATOM	3668	NE2	HIS	273	98.441	80.711	60.103	0.00	0.00	N
ATOM	3669	CD2	HIS	273	98.631	79.995	58.934	0.00	0.00	C
ATOM	3670	H	HIS	273	99.200	77.027	58.504	0.00	0.00	H
ATOM	3671	HA	HIS	273	101.491	77.482	56.535	0.00	0.00	H
ATOM	3672	1HB	HIS	273	99.904	79.300	56.580	0.00	0.00	H
ATOM	3673	2HB	HIS	273	101.478	79.808	57.111	0.00	0.00	H
ATOM	3674	HE1	HIS	273	99.988	81.567	61.300	0.00	0.00	H
ATOM	3675	HE2	HIS	273	97.590	81.135	60.489	0.00	0.00	H
ATOM	3676	HD2	HIS	273	97.843	79.641	58.283	0.00	0.00	H
ATOM	3677	N	ILE	274	102.221	76.650	59.534	1.00	0.00	N
ATOM	3678	CA	ILE	274	103.380	76.285	60.408	1.00	0.00	C
ATOM	3679	C	ILE	274	104.287	75.247	59.646	1.00	0.00	C
ATOM	3680	O	ILE	274	103.846	74.144	59.306	1.00	0.00	O
ATOM	3681	CB	ILE	274	102.859	75.786	61.818	1.00	0.00	C
ATOM	3682	CG1	ILE	274	102.352	76.893	62.794	1.00	0.00	C
ATOM	3683	CG2	ILE	274	103.914	74.996	62.640	1.00	0.00	C
ATOM	3684	CD1	ILE	274	101.144	77.724	62.340	1.00	0.00	C
ATOM	3685	H	ILE	274	101.319	76.162	59.609	1.00	0.00	H
ATOM	3686	HA	ILE	274	103.981	77.196	60.601	1.00	0.00	H
ATOM	3687	HB	ILE	274	102.021	75.081	61.635	1.00	0.00	H
ATOM	3688	1HG1	ILE	274	102.069	76.430	63.760	1.00	0.00	H
ATOM	3689	2HG1	ILE	274	103.185	77.575	63.045	1.00	0.00	H
ATOM	3690	2HG2	ILE	274	104.283	74.114	62.088	1.00	0.00	H
ATOM	3691	3HG2	ILE	274	104.802	75.606	62.892	1.00	0.00	H
ATOM	3692	1HG2	ILE	274	103.506	74.600	63.590	1.00	0.00	H
ATOM	3693	2HD1	ILE	274	101.395	78.386	61.491	1.00	0.00	H
ATOM	3694	3HD1	ILE	274	100.312	77.074	62.015	1.00	0.00	H
ATOM	3695	1HD1	ILE	274	100.765	78.375	63.149	1.00	0.00	H
ATOM	3696	N	ASN	275	105.570	75.583	59.420	1.00	0.00	N
ATOM	3697	CA	ASN	275	106.556	74.631	58.827	1.00	0.00	C
ATOM	3698	C	ASN	275	107.024	73.470	59.801	1.00	0.00	C
ATOM	3699	O	ASN	275	106.988	73.680	61.018	1.00	0.00	O
ATOM	3700	CB	ASN	275	107.707	75.475	58.199	1.00	0.00	C

ATOM	3701	CG	ASN	275	108.908	75.847	59.075	1.00	0.00	C
ATOM	3702	OD1	ASN	275	109.770	75.027	59.362	1.00	0.00	O
ATOM	3703	ND2	ASN	275	109.051	77.070	59.501	1.00	0.00	N
ATOM	3704	H	ASN	275	105.796	76.553	59.657	1.00	0.00	H
ATOM	3705	HA	ASN	275	106.038	74.137	57.980	1.00	0.00	H
ATOM	3706	1HB	ASN	275	108.130	74.902	57.357	1.00	0.00	H
ATOM	3707	2HB	ASN	275	107.304	76.377	57.702	1.00	0.00	H
ATOM	3708	1HD2	ASN	275	109.868	77.196	60.104	1.00	0.00	H
ATOM	3709	2HD2	ASN	275	108.261	77.716	59.370	1.00	0.00	H
ATOM	3710	N	PRO	276	107.529	72.281	59.351	1.00	0.00	N
ATOM	3711	CA	PRO	276	108.012	71.204	60.272	1.00	0.00	C
ATOM	3712	C	PRO	276	109.169	71.505	61.293	1.00	0.00	C
ATOM	3713	O	PRO	276	109.175	70.916	62.375	1.00	0.00	O
ATOM	3714	CB	PRO	276	108.317	70.048	59.295	1.00	0.00	C
ATOM	3715	CG	PRO	276	108.521	70.705	57.929	1.00	0.00	C
ATOM	3716	CD	PRO	276	107.552	71.883	57.930	1.00	0.00	C
ATOM	3717	HA	PRO	276	107.154	70.888	60.894	1.00	0.00	H
ATOM	3718	1HB	PRO	276	109.183	69.429	59.600	1.00	0.00	H
ATOM	3719	2HB	PRO	276	107.450	69.360	59.253	1.00	0.00	H
ATOM	3720	1HG	PRO	276	109.564	71.066	57.829	1.00	0.00	H
ATOM	3721	2HG	PRO	276	108.334	70.011	57.088	1.00	0.00	H
ATOM	3722	1HD	PRO	276	107.894	72.676	57.242	1.00	0.00	H
ATOM	3723	2HD	PRO	276	106.538	71.571	57.604	1.00	0.00	H
ATOM	3724	N	VAL	277	110.109	72.418	60.991	1.00	0.00	N
ATOM	3725	CA	VAL	277	111.112	72.927	61.992	1.00	0.00	C
ATOM	3726	C	VAL	277	110.471	73.844	63.108	1.00	0.00	C
ATOM	3727	O	VAL	277	110.775	73.669	64.292	1.00	0.00	O
ATOM	3728	CB	VAL	277	112.343	73.601	61.275	1.00	0.00	C
ATOM	3729	CG1	VAL	277	113.500	73.923	62.250	1.00	0.00	C
ATOM	3730	CG2	VAL	277	112.986	72.778	60.130	1.00	0.00	C
ATOM	3731	H	VAL	277	109.923	72.910	60.110	1.00	0.00	H
ATOM	3732	HA	VAL	277	111.515	72.046	62.533	1.00	0.00	H
ATOM	3733	HB	VAL	277	111.989	74.556	60.836	1.00	0.00	H
ATOM	3734	1HG1	VAL	277	113.946	73.012	62.689	1.00	0.00	H
ATOM	3735	2HG1	VAL	277	114.317	74.489	61.763	1.00	0.00	H
ATOM	3736	3HG1	VAL	277	113.158	74.543	63.096	1.00	0.00	H
ATOM	3737	2HG2	VAL	277	112.267	72.588	59.312	1.00	0.00	H
ATOM	3738	3HG2	VAL	277	113.844	73.303	59.667	1.00	0.00	H
ATOM	3739	1HG2	VAL	277	113.347	71.793	60.477	1.00	0.00	H
ATOM	3740	N	ALA	278	109.573	74.787	62.751	1.00	0.00	N
ATOM	3741	CA	ALA	278	108.679	75.464	63.733	1.00	0.00	C
ATOM	3742	C	ALA	278	107.712	74.540	64.557	1.00	0.00	C
ATOM	3743	O	ALA	278	107.630	74.703	65.775	1.00	0.00	O
ATOM	3744	CB	ALA	278	107.921	76.556	62.955	1.00	0.00	C
ATOM	3745	H	ALA	278	109.333	74.738	61.754	1.00	0.00	H
ATOM	3746	HA	ALA	278	109.320	75.978	64.478	1.00	0.00	H
ATOM	3747	2HB	ALA	278	108.606	77.275	62.472	1.00	0.00	H
ATOM	3748	3HB	ALA	278	107.273	76.132	62.163	1.00	0.00	H
ATOM	3749	1HB	ALA	278	107.267	77.145	63.624	1.00	0.00	H
ATOM	3750	N	ALA	279	107.026	73.560	63.934	1.00	0.00	N
ATOM	3751	CA	ALA	279	106.300	72.479	64.659	1.00	0.00	C
ATOM	3752	C	ALA	279	107.139	71.631	65.676	1.00	0.00	C
ATOM	3753	O	ALA	279	106.714	71.487	66.822	1.00	0.00	O
ATOM	3754	CB	ALA	279	105.640	71.588	63.591	1.00	0.00	C
ATOM	3755	H	ALA	279	107.144	73.548	62.910	1.00	0.00	H
ATOM	3756	HA	ALA	279	105.486	72.953	65.245	1.00	0.00	H
ATOM	3757	2HB	ALA	279	105.033	72.162	62.868	1.00	0.00	H
ATOM	3758	3HB	ALA	279	106.390	71.021	63.011	1.00	0.00	H
ATOM	3759	1HB	ALA	279	104.968	70.841	64.053	1.00	0.00	H
ATOM	3760	N	SER	280	108.335	71.141	65.295	1.00	0.00	N
ATOM	3761	CA	SER	280	109.313	70.538	66.246	1.00	0.00	C
ATOM	3762	C	SER	280	109.736	71.432	67.466	1.00	0.00	C
ATOM	3763	O	SER	280	109.698	70.949	68.596	1.00	0.00	O
ATOM	3764	CB	SER	280	110.530	70.068	65.414	1.00	0.00	C
ATOM	3765	OG	SER	280	111.472	69.355	66.219	1.00	0.00	O
ATOM	3766	H	SER	280	108.550	71.281	64.299	1.00	0.00	H
ATOM	3767	HA	SER	280	108.843	69.630	66.675	1.00	0.00	H
ATOM	3768	1HB	SER	280	110.202	69.410	64.585	1.00	0.00	H
ATOM	3769	2HB	SER	280	111.030	70.929	64.926	1.00	0.00	H
ATOM	3770	HG	SER	280	111.677	69.903	66.986	1.00	0.00	H
ATOM	3771	N	LEU	281	110.091	72.716	67.265	0.00	0.00	N
ATOM	3772	CA	LEU	281	110.282	73.690	68.385	0.00	0.00	C
ATOM	3773	C	LEU	281	109.019	73.976	69.287	0.00	0.00	C

ATOM	3774	O	LEU	281	109.153	74.008	70.512	0.00	0.00	O
ATOM	3775	CB	LEU	281	110.916	74.971	67.767	0.00	0.00	C
ATOM	3776	CG	LEU	281	111.466	76.022	68.769	0.00	0.00	C
ATOM	3777	CD1	LEU	281	112.724	75.538	69.510	0.00	0.00	C
ATOM	3778	CD2	LEU	281	111.794	77.333	68.038	0.00	0.00	C
ATOM	3779	H	LEU	281	110.044	73.008	66.280	0.00	0.00	H
ATOM	3780	HA	LEU	281	111.034	73.249	69.067	0.00	0.00	H
ATOM	3781	1HB	LEU	281	110.155	75.447	67.118	0.00	0.00	H
ATOM	3782	2HB	LEU	281	111.735	74.695	67.073	0.00	0.00	H
ATOM	3783	HG	LEU	281	110.686	76.238	69.526	0.00	0.00	H
ATOM	3784	1HD1	LEU	281	113.118	76.305	70.202	0.00	0.00	H
ATOM	3785	2HD1	LEU	281	112.523	74.639	70.123	0.00	0.00	H
ATOM	3786	3HD1	LEU	281	113.541	75.285	68.812	0.00	0.00	H
ATOM	3787	1HD2	LEU	281	112.150	78.116	68.736	0.00	0.00	H
ATOM	3788	2HD2	LEU	281	112.581	77.195	67.273	0.00	0.00	H
ATOM	3789	3HD2	LEU	281	110.909	77.749	67.522	0.00	0.00	H
ATOM	3790	N	ILE	282	107.811	74.141	68.710	1.00	0.00	N
ATOM	3791	CA	ILE	282	106.519	74.183	69.481	1.00	0.00	C
ATOM	3792	C	ILE	282	106.240	72.868	70.311	1.00	0.00	C
ATOM	3793	O	ILE	282	105.937	72.968	71.499	1.00	0.00	O
ATOM	3794	CB	ILE	282	105.333	74.624	68.532	1.00	0.00	C
ATOM	3795	CG1	ILE	282	105.508	76.060	67.944	1.00	0.00	C
ATOM	3796	CG2	ILE	282	103.939	74.566	69.215	1.00	0.00	C
ATOM	3797	CD1	ILE	282	104.640	76.398	66.716	1.00	0.00	C
ATOM	3798	H	ILE	282	107.829	74.102	67.681	1.00	0.00	H
ATOM	3799	HA	ILE	282	106.618	74.980	70.244	1.00	0.00	H
ATOM	3800	HB	ILE	282	105.319	73.908	67.686	1.00	0.00	H
ATOM	3801	1HG1	ILE	282	105.354	76.820	68.735	1.00	0.00	H
ATOM	3802	2HG1	ILE	282	106.559	76.201	67.631	1.00	0.00	H
ATOM	3803	2HG2	ILE	282	103.703	73.553	69.590	1.00	0.00	H
ATOM	3804	3HG2	ILE	282	103.874	75.257	70.076	1.00	0.00	H
ATOM	3805	1HG2	ILE	282	103.116	74.826	68.525	1.00	0.00	H
ATOM	3806	2HD1	ILE	282	104.804	75.679	65.892	1.00	0.00	H
ATOM	3807	3HD1	ILE	282	103.559	76.401	66.950	1.00	0.00	H
ATOM	3808	1HD1	ILE	282	104.881	77.403	66.322	1.00	0.00	H
ATOM	3809	N	GLN	283	106.365	71.662	69.727	1.00	0.00	N
ATOM	3810	CA	GLN	283	106.324	70.366	70.478	1.00	0.00	C
ATOM	3811	C	GLN	283	107.407	70.164	71.602	1.00	0.00	C
ATOM	3812	O	GLN	283	107.077	69.647	72.669	1.00	0.00	O
ATOM	3813	CB	GLN	283	106.371	69.207	69.441	1.00	0.00	C
ATOM	3814	CG	GLN	283	105.123	69.066	68.524	1.00	0.00	C
ATOM	3815	CD	GLN	283	105.263	67.998	67.437	1.00	0.00	C
ATOM	3816	OE1	GLN	283	105.841	68.208	66.378	1.00	0.00	O
ATOM	3817	NE2	GLN	283	104.736	66.821	67.648	1.00	0.00	N
ATOM	3818	H	GLN	283	106.619	71.701	68.728	1.00	0.00	H
ATOM	3819	HA	GLN	283	105.351	70.309	71.006	1.00	0.00	H
ATOM	3820	1HB	GLN	283	107.284	69.312	68.820	1.00	0.00	H
ATOM	3821	2HB	GLN	283	106.509	68.248	69.979	1.00	0.00	H
ATOM	3822	1HG	GLN	283	104.215	68.892	69.130	1.00	0.00	H
ATOM	3823	2HG	GLN	283	104.931	70.020	68.000	1.00	0.00	H
ATOM	3824	1HE2	GLN	283	104.316	66.660	68.566	1.00	0.00	H
ATOM	3825	2HE2	GLN	283	104.911	66.152	66.894	1.00	0.00	H
ATOM	3826	N	LYS	284	108.670	70.582	71.395	1.00	0.00	N
ATOM	3827	CA	LYS	284	109.702	70.663	72.477	1.00	0.00	C
ATOM	3828	C	LYS	284	109.350	71.603	73.689	1.00	0.00	C
ATOM	3829	O	LYS	284	109.483	71.189	74.843	1.00	0.00	O
ATOM	3830	CB	LYS	284	111.052	71.077	71.820	1.00	0.00	C
ATOM	3831	CG	LYS	284	111.752	69.995	70.965	1.00	0.00	C
ATOM	3832	CD	LYS	284	112.939	70.569	70.164	1.00	0.00	C
ATOM	3833	CE	LYS	284	113.574	69.518	69.246	1.00	0.00	C
ATOM	3834	NZ	LYS	284	114.669	70.131	68.468	1.00	0.00	N
ATOM	3835	1HZ	LYS	284	115.093	69.421	67.853	1.00	0.00	H
ATOM	3836	2HZ	LYS	284	114.295	70.901	67.895	1.00	0.00	H
ATOM	3837	3HZ	LYS	284	115.385	70.498	69.111	1.00	0.00	H
ATOM	3838	H	LYS	284	108.845	70.927	70.442	1.00	0.00	H
ATOM	3839	HA	LYS	284	109.825	69.652	72.914	1.00	0.00	H
ATOM	3840	1HB	LYS	284	110.891	71.994	71.217	1.00	0.00	H
ATOM	3841	2HB	LYS	284	111.762	71.394	72.606	1.00	0.00	H
ATOM	3842	1HG	LYS	284	112.088	69.161	71.612	1.00	0.00	H
ATOM	3843	2HG	LYS	284	111.023	69.541	70.266	1.00	0.00	H
ATOM	3844	1HD	LYS	284	112.585	71.426	69.555	1.00	0.00	H
ATOM	3845	2HD	LYS	284	113.695	70.985	70.860	1.00	0.00	H
ATOM	3846	1HE	LYS	284	113.956	68.663	69.840	1.00	0.00	H

ATOM	3847	2HE	LYS	284	112.813	69.091	68.562	1.00	0.00	H
ATOM	3848	N	MET	285	108.903	72.845	73.438	1.00	0.00	N
ATOM	3849	CA	MET	285	108.343	73.747	74.490	1.00	0.00	C
ATOM	3850	C	MET	285	107.007	73.268	75.172	1.00	0.00	C
ATOM	3851	O	MET	285	106.880	73.356	76.396	1.00	0.00	O
ATOM	3852	CB	MET	285	108.192	75.163	73.863	1.00	0.00	C
ATOM	3853	CG	MET	285	109.509	75.909	73.553	1.00	0.00	C
ATOM	3854	SD	MET	285	109.147	77.567	72.955	1.00	0.00	S
ATOM	3855	CE	MET	285	110.808	78.115	72.529	1.00	0.00	C
ATOM	3856	H	MET	285	108.820	73.061	72.436	1.00	0.00	H
ATOM	3857	HA	MET	285	109.080	73.822	75.315	1.00	0.00	H
ATOM	3858	1HB	MET	285	107.573	75.105	72.945	1.00	0.00	H
ATOM	3859	2HB	MET	285	107.603	75.796	74.550	1.00	0.00	H
ATOM	3860	1HG	MET	285	110.149	75.976	74.452	1.00	0.00	H
ATOM	3861	2HG	MET	285	110.091	75.364	72.785	1.00	0.00	H
ATOM	3862	1HE	MET	285	111.438	78.200	73.430	1.00	0.00	H
ATOM	3863	3HE	MET	285	111.288	77.407	71.829	1.00	0.00	H
ATOM	3864	2HE	MET	285	110.774	79.105	72.043	1.00	0.00	H
ATOM	3865	N	LEU	286	106.023	72.769	74.403	0.00	0.00	N
ATOM	3866	CA	LEU	286	104.734	72.249	74.938	0.00	0.00	C
ATOM	3867	C	LEU	286	104.765	70.689	75.136	0.00	0.00	C
ATOM	3868	O	LEU	286	104.191	69.933	74.344	0.00	0.00	O
ATOM	3869	CB	LEU	286	103.593	72.713	73.979	0.00	0.00	C
ATOM	3870	CG	LEU	286	103.350	74.234	73.781	0.00	0.00	C
ATOM	3871	CD1	LEU	286	102.345	74.488	72.647	0.00	0.00	C
ATOM	3872	CD2	LEU	286	102.828	74.911	75.053	0.00	0.00	C
ATOM	3873	H	LEU	286	106.248	72.721	73.399	0.00	0.00	H
ATOM	3874	HA	LEU	286	104.520	72.696	75.927	0.00	0.00	H
ATOM	3875	1HB	LEU	286	102.649	72.257	74.326	0.00	0.00	H
ATOM	3876	2HB	LEU	286	103.772	72.247	72.989	0.00	0.00	H
ATOM	3877	HG	LEU	286	104.310	74.702	73.489	0.00	0.00	H
ATOM	3878	1HD1	LEU	286	102.251	75.564	72.415	0.00	0.00	H
ATOM	3879	2HD1	LEU	286	102.649	73.981	71.715	0.00	0.00	H
ATOM	3880	3HD1	LEU	286	101.334	74.117	72.893	0.00	0.00	H
ATOM	3881	1HD2	LEU	286	102.662	75.994	74.907	0.00	0.00	H
ATOM	3882	2HD2	LEU	286	101.871	74.475	75.399	0.00	0.00	H
ATOM	3883	3HD2	LEU	286	103.544	74.819	75.886	0.00	0.00	H
ATOM	3884	N	GLN	287	105.413	70.203	76.211	0.00	0.00	N
ATOM	3885	CA	GLN	287	105.589	68.743	76.475	0.00	0.00	C
ATOM	3886	C	GLN	287	105.173	68.375	77.939	0.00	0.00	C
ATOM	3887	O	GLN	287	105.882	68.685	78.895	0.00	0.00	O
ATOM	3888	CB	GLN	287	107.068	68.397	76.131	0.00	0.00	C
ATOM	3889	CG	GLN	287	107.540	66.935	76.360	0.00	0.00	C
ATOM	3890	CD	GLN	287	106.894	65.837	75.513	0.00	0.00	C
ATOM	3891	OE1	GLN	287	107.388	65.437	74.467	0.00	0.00	O
ATOM	3892	NE2	GLN	287	105.791	65.276	75.937	0.00	0.00	N
ATOM	3893	H	GLN	287	105.978	70.908	76.702	0.00	0.00	H
ATOM	3894	HA	GLN	287	104.957	68.147	75.785	0.00	0.00	H
ATOM	3895	1HB	GLN	287	107.737	69.060	76.715	0.00	0.00	H
ATOM	3896	2HB	GLN	287	107.271	68.671	75.076	0.00	0.00	H
ATOM	3897	1HG	GLN	287	107.477	66.675	77.433	0.00	0.00	H
ATOM	3898	2HG	GLN	287	108.623	66.896	76.145	0.00	0.00	H
ATOM	3899	1HE2	GLN	287	105.310	65.754	76.700	0.00	0.00	H
ATOM	3900	2HE2	GLN	287	105.393	64.634	75.247	0.00	0.00	H
ATOM	3901	N	THR	288	104.048	67.664	78.139	1.00	0.00	N
ATOM	3902	CA	THR	288	103.543	67.291	79.511	1.00	0.00	C
ATOM	3903	C	THR	288	104.436	66.358	80.418	1.00	0.00	C
ATOM	3904	O	THR	288	104.234	66.308	81.634	1.00	0.00	O
ATOM	3905	CB	THR	288	102.058	66.822	79.390	1.00	0.00	C
ATOM	3906	OG1	THR	288	101.424	66.860	80.660	1.00	0.00	O
ATOM	3907	CG2	THR	288	101.822	65.403	78.845	1.00	0.00	C
ATOM	3908	H	THR	288	103.483	67.504	77.290	1.00	0.00	H
ATOM	3909	HA	THR	288	103.495	68.235	80.088	1.00	0.00	H
ATOM	3910	HB	THR	288	101.518	67.539	78.739	1.00	0.00	H
ATOM	3911	HG1	THR	288	100.655	66.284	80.589	1.00	0.00	H
ATOM	3912	1HG2	THR	288	100.743	65.181	78.732	1.00	0.00	H
ATOM	3913	2HG2	THR	288	102.281	65.264	77.849	1.00	0.00	H
ATOM	3914	3HG2	THR	288	102.250	64.629	79.511	1.00	0.00	H
ATOM	3915	N	ASP	289	105.434	65.659	79.851	0.00	0.00	N
ATOM	3916	CA	ASP	289	106.531	65.022	80.628	0.00	0.00	C
ATOM	3917	C	ASP	289	107.747	66.022	80.745	0.00	0.00	C
ATOM	3918	O	ASP	289	108.507	66.112	79.773	0.00	0.00	O
ATOM	3919	CB	ASP	289	106.933	63.698	79.922	0.00	0.00	C

ATOM	3920	CG	ASP	289	105.899	62.579	79.992	0.00	0.00	C
ATOM	3921	OD1	ASP	289	105.743	61.857	80.970	0.00	0.00	O
ATOM	3922	OD2	ASP	289	105.173	62.469	78.848	0.00	0.00	O
ATOM	3923	H	ASP	289	105.566	65.931	78.873	0.00	0.00	H
ATOM	3924	HA	ASP	289	106.183	64.747	81.643	0.00	0.00	H
ATOM	3925	1HB	ASP	289	107.856	63.302	80.382	0.00	0.00	H
ATOM	3926	2HB	ASP	289	107.206	63.884	78.866	0.00	0.00	H
ATOM	3927	N	PRO	290	108.009	66.769	81.862	1.00	0.00	N
ATOM	3928	CA	PRO	290	109.137	67.754	81.926	1.00	0.00	C
ATOM	3929	C	PRO	290	110.615	67.241	81.787	1.00	0.00	C
ATOM	3930	O	PRO	290	111.483	68.016	81.382	1.00	0.00	O
ATOM	3931	CB	PRO	290	108.847	68.505	83.240	1.00	0.00	C
ATOM	3932	CG	PRO	290	107.998	67.547	84.076	1.00	0.00	C
ATOM	3933	CD	PRO	290	107.135	66.813	83.051	1.00	0.00	C
ATOM	3934	HA	PRO	290	109.003	68.477	81.096	1.00	0.00	H
ATOM	3935	1HB	PRO	290	109.761	68.838	83.770	1.00	0.00	H
ATOM	3936	2HB	PRO	290	108.273	69.427	83.016	1.00	0.00	H
ATOM	3937	1HG	PRO	290	108.650	66.830	84.612	1.00	0.00	H
ATOM	3938	2HG	PRO	290	107.394	68.066	84.842	1.00	0.00	H
ATOM	3939	1HD	PRO	290	106.837	65.816	83.426	1.00	0.00	H
ATOM	3940	2HD	PRO	290	106.212	67.384	82.828	1.00	0.00	H
ATOM	3941	N	THR	291	110.902	65.954	82.033	0.00	0.00	N
ATOM	3942	CA	THR	291	112.170	65.287	81.572	0.00	0.00	C
ATOM	3943	C	THR	291	112.443	65.277	80.021	0.00	0.00	C
ATOM	3944	O	THR	291	113.599	65.396	79.608	0.00	0.00	O
ATOM	3945	CB	THR	291	112.272	63.838	82.150	0.00	0.00	C
ATOM	3946	OG1	THR	291	111.144	63.050	81.782	0.00	0.00	O
ATOM	3947	CG2	THR	291	112.401	63.745	83.679	0.00	0.00	C
ATOM	3948	H	THR	291	110.076	65.407	82.290	0.00	0.00	H
ATOM	3949	HA	THR	291	113.018	65.861	81.998	0.00	0.00	H
ATOM	3950	HB	THR	291	113.182	63.366	81.723	0.00	0.00	H
ATOM	3951	HG1	THR	291	111.255	62.203	82.220	0.00	0.00	H
ATOM	3952	1HG2	THR	291	112.536	62.702	84.020	0.00	0.00	H
ATOM	3953	2HG2	THR	291	113.270	64.321	84.048	0.00	0.00	H
ATOM	3954	3HG2	THR	291	111.506	64.145	84.192	0.00	0.00	H
ATOM	3955	N	ALA	292	111.407	65.155	79.170	1.00	0.00	N
ATOM	3956	CA	ALA	292	111.517	65.430	77.707	1.00	0.00	C
ATOM	3957	C	ALA	292	111.351	66.921	77.217	1.00	0.00	C
ATOM	3958	O	ALA	292	111.419	67.163	76.008	1.00	0.00	O
ATOM	3959	CB	ALA	292	110.464	64.496	77.075	1.00	0.00	C
ATOM	3960	H	ALA	292	110.496	65.160	79.642	1.00	0.00	H
ATOM	3961	HA	ALA	292	112.511	65.107	77.339	1.00	0.00	H
ATOM	3962	2HB	ALA	292	110.646	63.432	77.318	1.00	0.00	H
ATOM	3963	3HB	ALA	292	109.436	64.743	77.400	1.00	0.00	H
ATOM	3964	1HB	ALA	292	110.472	64.572	75.971	1.00	0.00	H
ATOM	3965	N	ARG	293	111.155	67.913	78.102	0.00	0.00	N
ATOM	3966	CA	ARG	293	111.035	69.349	77.730	0.00	0.00	C
ATOM	3967	C	ARG	293	112.431	70.079	77.848	0.00	0.00	C
ATOM	3968	O	ARG	293	112.874	70.307	78.980	0.00	0.00	O
ATOM	3969	CB	ARG	293	109.945	69.948	78.668	0.00	0.00	C
ATOM	3970	CG	ARG	293	109.355	71.322	78.250	0.00	0.00	C
ATOM	3971	CD	ARG	293	108.545	72.043	79.350	0.00	0.00	C
ATOM	3972	NE	ARG	293	107.377	71.246	79.800	0.00	0.00	N
ATOM	3973	CZ	ARG	293	106.613	71.500	80.849	0.00	0.00	C
ATOM	3974	NH1	ARG	293	106.746	72.531	81.627	0.00	0.00	N
ATOM	3975	NH2	ARG	293	105.679	70.655	81.106	0.00	0.00	N
ATOM	3976	HE	ARG	293	107.138	70.414	79.242	1.00	0.00	H
ATOM	3977	H	ARG	293	111.190	67.608	79.081	0.00	0.00	H
ATOM	3978	HA	ARG	293	110.638	69.440	76.702	0.00	0.00	H
ATOM	3979	1HB	ARG	293	110.346	70.018	79.696	0.00	0.00	H
ATOM	3980	2HB	ARG	293	109.087	69.250	78.757	0.00	0.00	H
ATOM	3981	1HG	ARG	293	108.717	71.197	77.352	0.00	0.00	H
ATOM	3982	2HG	ARG	293	110.172	71.994	77.921	0.00	0.00	H
ATOM	3983	1HD	ARG	293	108.180	73.013	78.961	0.00	0.00	H
ATOM	3984	2HD	ARG	293	109.216	72.282	80.197	0.00	0.00	H
ATOM	3985	1HH1	ARG	293	106.110	72.599	82.417	0.00	0.00	H
ATOM	3986	2HH1	ARG	293	107.501	73.161	81.338	0.00	0.00	H
ATOM	3987	1HH2	ARG	293	105.098	70.793	81.925	0.00	0.00	H
ATOM	3988	2HH2	ARG	293	105.711	69.884	80.425	0.00	0.00	H
ATOM	3989	N	PRO	294	113.176	70.471	76.769	1.00	0.00	N
ATOM	3990	CA	PRO	294	114.485	71.175	76.914	1.00	0.00	C
ATOM	3991	C	PRO	294	114.392	72.639	77.466	1.00	0.00	C
ATOM	3992	O	PRO	294	113.468	73.393	77.152	1.00	0.00	O

ATOM	3993	CB	PRO	294	115.049	71.081	75.481	1.00	0.00	C
ATOM	3994	CG	PRO	294	113.832	70.955	74.566	1.00	0.00	C
ATOM	3995	CD	PRO	294	112.832	70.136	75.375	1.00	0.00	C
ATOM	3996	HA	PRO	294	115.134	70.581	77.588	1.00	0.00	H
ATOM	3997	1HB	PRO	294	115.680	71.944	75.202	1.00	0.00	H
ATOM	3998	2HB	PRO	294	115.686	70.180	75.389	1.00	0.00	H
ATOM	3999	1HG	PRO	294	113.411	71.958	74.363	1.00	0.00	H
ATOM	4000	2HG	PRO	294	114.067	70.495	73.588	1.00	0.00	H
ATOM	4001	1HD	PRO	294	111.795	70.403	75.105	1.00	0.00	H
ATOM	4002	2HD	PRO	294	112.957	69.050	75.192	1.00	0.00	H
ATOM	4003	N	THR	295	115.339	73.037	78.328	1.00	0.00	N
ATOM	4004	CA	THR	295	115.353	74.386	78.981	1.00	0.00	C
ATOM	4005	C	THR	295	116.817	74.695	79.466	1.00	0.00	C
ATOM	4006	O	THR	295	117.387	73.917	80.231	1.00	0.00	O
ATOM	4007	CB	THR	295	114.333	74.468	80.166	1.00	0.00	C
ATOM	4008	OG1	THR	295	113.010	74.194	79.725	1.00	0.00	O
ATOM	4009	CG2	THR	295	114.231	75.846	80.832	1.00	0.00	C
ATOM	4010	H	THR	295	116.015	72.303	78.578	1.00	0.00	H
ATOM	4011	HA	THR	295	115.040	75.133	78.232	1.00	0.00	H
ATOM	4012	HB	THR	295	114.610	73.714	80.932	1.00	0.00	H
ATOM	4013	HG1	THR	295	113.092	73.632	78.939	1.00	0.00	H
ATOM	4014	1HG2	THR	295	113.968	76.636	80.108	1.00	0.00	H
ATOM	4015	2HG2	THR	295	113.451	75.851	81.616	1.00	0.00	H
ATOM	4016	3HG2	THR	295	115.181	76.140	81.311	1.00	0.00	H
ATOM	4017	N	ILE	296	117.571	75.760	79.174	1.00	0.00	N
ATOM	4018	CA	ILE	296	117.200	76.943	78.320	1.00	0.00	C
ATOM	4019	C	ILE	296	118.198	77.193	77.130	1.00	0.00	C
ATOM	4020	O	ILE	296	117.754	77.424	76.002	1.00	0.00	O
ATOM	4021	CB	ILE	296	116.909	78.203	79.219	1.00	0.00	C
ATOM	4022	CG1	ILE	296	116.285	79.421	78.478	1.00	0.00	C
ATOM	4023	CG2	ILE	296	118.123	78.712	80.038	1.00	0.00	C
ATOM	4024	CD1	ILE	296	114.886	79.182	77.886	1.00	0.00	C
ATOM	4025	H	ILE	296	118.460	75.689	79.683	1.00	0.00	H
ATOM	4026	HA	ILE	296	116.253	76.730	77.797	1.00	0.00	H
ATOM	4027	HB	ILE	296	116.153	77.880	79.960	1.00	0.00	H
ATOM	4028	1HG1	ILE	296	116.200	80.276	79.177	1.00	0.00	H
ATOM	4029	2HG1	ILE	296	116.970	79.783	77.684	1.00	0.00	H
ATOM	4030	2HG2	ILE	296	118.571	77.916	80.662	1.00	0.00	H
ATOM	4031	3HG2	ILE	296	118.925	79.109	79.388	1.00	0.00	H
ATOM	4032	1HG2	ILE	296	117.843	79.526	80.735	1.00	0.00	H
ATOM	4033	2HD1	ILE	296	114.897	78.440	77.066	1.00	0.00	H
ATOM	4034	3HD1	ILE	296	114.170	78.831	78.652	1.00	0.00	H
ATOM	4035	1HD1	ILE	296	114.472	80.115	77.461	1.00	0.00	H
ATOM	4036	N	ASN	297	119.524	77.082	77.342	1.00	0.00	N
ATOM	4037	CA	ASN	297	120.539	76.963	76.244	1.00	0.00	C
ATOM	4038	C	ASN	297	120.318	75.865	75.137	1.00	0.00	C
ATOM	4039	O	ASN	297	120.720	76.074	73.993	1.00	0.00	O
ATOM	4040	CB	ASN	297	121.955	76.877	76.885	1.00	0.00	C
ATOM	4041	CG	ASN	297	122.271	75.635	77.728	1.00	0.00	C
ATOM	4042	OD1	ASN	297	121.591	75.318	78.696	1.00	0.00	O
ATOM	4043	ND2	ASN	297	123.300	74.896	77.410	1.00	0.00	N
ATOM	4044	H	ASN	297	119.777	76.885	78.316	1.00	0.00	H
ATOM	4045	HA	ASN	297	120.509	77.926	75.696	1.00	0.00	H
ATOM	4046	1HB	ASN	297	122.710	77.007	76.087	1.00	0.00	H
ATOM	4047	2HB	ASN	297	122.116	77.751	77.540	1.00	0.00	H
ATOM	4048	1HD2	ASN	297	123.467	74.122	78.059	1.00	0.00	H
ATOM	4049	2HD2	ASN	297	123.883	75.208	76.631	1.00	0.00	H
ATOM	4050	N	GLU	298	119.665	74.735	75.458	1.00	0.00	N
ATOM	4051	CA	GLU	298	119.131	73.759	74.458	1.00	0.00	C
ATOM	4052	C	GLU	298	118.095	74.333	73.417	1.00	0.00	C
ATOM	4053	O	GLU	298	118.223	74.070	72.223	1.00	0.00	O
ATOM	4054	CB	GLU	298	118.500	72.576	75.246	1.00	0.00	C
ATOM	4055	CG	GLU	298	119.433	71.725	76.149	1.00	0.00	C
ATOM	4056	CD	GLU	298	118.675	70.676	76.962	1.00	0.00	C
ATOM	4057	OE1	GLU	298	117.817	70.947	77.795	1.00	0.00	O
ATOM	4058	OE2	GLU	298	119.052	69.407	76.656	1.00	0.00	O
ATOM	4059	H	GLU	298	119.435	74.674	76.456	1.00	0.00	H
ATOM	4060	HA	GLU	298	119.980	73.366	73.862	1.00	0.00	H
ATOM	4061	1HB	GLU	298	117.661	72.964	75.858	1.00	0.00	H
ATOM	4062	2HB	GLU	298	118.022	71.888	74.519	1.00	0.00	H
ATOM	4063	1HG	GLU	298	120.219	71.239	75.542	1.00	0.00	H
ATOM	4064	2HG	GLU	298	119.971	72.366	76.871	1.00	0.00	H
ATOM	4065	N	LEU	299	117.091	75.115	73.859	1.00	0.00	N

ATOM	4066	CA	LEU	299	116.186	75.882	72.942	1.00	0.00	C
ATOM	4067	C	LEU	299	116.861	77.050	72.136	1.00	0.00	C
ATOM	4068	O	LEU	299	116.532	77.249	70.965	1.00	0.00	O
ATOM	4069	CB	LEU	299	114.977	76.408	73.767	1.00	0.00	C
ATOM	4070	CG	LEU	299	113.984	75.356	74.328	1.00	0.00	C
ATOM	4071	CD1	LEU	299	113.061	76.019	75.358	1.00	0.00	C
ATOM	4072	CD2	LEU	299	113.127	74.708	73.229	1.00	0.00	C
ATOM	4073	H	LEU	299	117.153	75.335	74.857	1.00	0.00	H
ATOM	4074	HA	LEU	299	115.798	75.187	72.171	1.00	0.00	H
ATOM	4075	1HB	LEU	299	115.370	77.032	74.594	1.00	0.00	H
ATOM	4076	2HB	LEU	299	114.398	77.123	73.148	1.00	0.00	H
ATOM	4077	HG	LEU	299	114.545	74.556	74.851	1.00	0.00	H
ATOM	4078	2HD1	LEU	299	113.638	76.425	76.207	1.00	0.00	H
ATOM	4079	3HD1	LEU	299	112.472	76.850	74.931	1.00	0.00	H
ATOM	4080	1HD1	LEU	299	112.342	75.295	75.786	1.00	0.00	H
ATOM	4081	2HD2	LEU	299	112.564	75.457	72.642	1.00	0.00	H
ATOM	4082	3HD2	LEU	299	113.738	74.125	72.517	1.00	0.00	H
ATOM	4083	1HD2	LEU	299	112.380	74.008	73.649	1.00	0.00	H
ATOM	4084	N	LEU	300	117.800	77.804	72.742	0.00	0.00	N
ATOM	4085	CA	LEU	300	118.689	78.749	72.003	0.00	0.00	C
ATOM	4086	C	LEU	300	119.619	78.094	70.910	0.00	0.00	C
ATOM	4087	O	LEU	300	119.696	78.602	69.791	0.00	0.00	O
ATOM	4088	CB	LEU	300	119.475	79.548	73.087	0.00	0.00	C
ATOM	4089	CG	LEU	300	120.146	80.865	72.617	0.00	0.00	C
ATOM	4090	CD1	LEU	300	119.115	81.989	72.419	0.00	0.00	C
ATOM	4091	CD2	LEU	300	121.191	81.327	73.645	0.00	0.00	C
ATOM	4092	H	LEU	300	117.959	77.545	73.722	0.00	0.00	H
ATOM	4093	HA	LEU	300	118.035	79.456	71.458	0.00	0.00	H
ATOM	4094	1HB	LEU	300	120.243	78.874	73.511	0.00	0.00	H
ATOM	4095	2HB	LEU	300	118.821	79.790	73.950	0.00	0.00	H
ATOM	4096	HG	LEU	300	120.669	80.685	71.654	0.00	0.00	H
ATOM	4097	1HD1	LEU	300	119.592	82.917	72.055	0.00	0.00	H
ATOM	4098	2HD1	LEU	300	118.343	81.724	71.675	0.00	0.00	H
ATOM	4099	3HD1	LEU	300	118.589	82.249	73.357	0.00	0.00	H
ATOM	4100	1HD2	LEU	300	121.695	82.259	73.327	0.00	0.00	H
ATOM	4101	2HD2	LEU	300	120.746	81.517	74.640	0.00	0.00	H
ATOM	4102	3HD2	LEU	300	121.988	80.573	73.783	0.00	0.00	H
ATOM	4103	N	ASN	301	120.297	76.970	71.206	1.00	0.00	N
ATOM	4104	CA	ASN	301	121.104	76.208	70.204	1.00	0.00	C
ATOM	4105	C	ASN	301	120.227	75.154	69.432	1.00	0.00	C
ATOM	4106	O	ASN	301	120.271	73.949	69.696	1.00	0.00	O
ATOM	4107	CB	ASN	301	122.318	75.573	70.940	1.00	0.00	C
ATOM	4108	CG	ASN	301	123.381	76.548	71.451	1.00	0.00	C
ATOM	4109	OD1	ASN	301	124.255	77.005	70.727	1.00	0.00	O
ATOM	4110	ND2	ASN	301	123.349	76.909	72.706	1.00	0.00	N
ATOM	4111	H	ASN	301	120.089	76.589	72.137	1.00	0.00	H
ATOM	4112	HA	ASN	301	121.521	76.899	69.441	1.00	0.00	H
ATOM	4113	1HB	ASN	301	121.973	74.907	71.753	1.00	0.00	H
ATOM	4114	2HB	ASN	301	122.841	74.896	70.241	1.00	0.00	H
ATOM	4115	1HD2	ASN	301	124.007	77.663	72.912	1.00	0.00	H
ATOM	4116	2HD2	ASN	301	122.480	76.659	73.193	1.00	0.00	H
ATOM	4117	N	ASP	302	119.431	75.633	68.462	1.00	0.00	N
ATOM	4118	CA	ASP	302	118.470	74.800	67.682	1.00	0.00	C
ATOM	4119	C	ASP	302	118.558	75.124	66.146	1.00	0.00	C
ATOM	4120	O	ASP	302	118.888	76.244	65.746	1.00	0.00	O
ATOM	4121	CB	ASP	302	117.068	75.070	68.304	1.00	0.00	C
ATOM	4122	CG	ASP	302	115.930	74.205	67.769	1.00	0.00	C
ATOM	4123	OD1	ASP	302	115.315	74.453	66.736	1.00	0.00	O
ATOM	4124	OD2	ASP	302	115.684	73.122	68.555	1.00	0.00	O
ATOM	4125	H	ASP	302	119.450	76.657	68.388	1.00	0.00	H
ATOM	4126	HA	ASP	302	118.713	73.724	67.810	1.00	0.00	H
ATOM	4127	1HB	ASP	302	117.108	74.932	69.403	1.00	0.00	H
ATOM	4128	2HB	ASP	302	116.784	76.131	68.168	1.00	0.00	H
ATOM	4129	N	GLU	303	118.186	74.166	65.272	1.00	0.00	N
ATOM	4130	CA	GLU	303	118.106	74.393	63.789	1.00	0.00	C
ATOM	4131	C	GLU	303	117.247	75.612	63.272	1.00	0.00	C
ATOM	4132	O	GLU	303	117.653	76.272	62.311	1.00	0.00	O
ATOM	4133	CB	GLU	303	117.698	73.037	63.143	1.00	0.00	C
ATOM	4134	CG	GLU	303	117.791	72.950	61.594	1.00	0.00	C
ATOM	4135	CD	GLU	303	119.196	73.093	61.008	1.00	0.00	C
ATOM	4136	OE1	GLU	303	120.002	72.174	60.934	1.00	0.00	O
ATOM	4137	OE2	GLU	303	119.453	74.358	60.580	1.00	0.00	O
ATOM	4138	H	GLU	303	117.932	73.274	65.704	1.00	0.00	H

ATOM	4139	HA	GLU	303	119.138	74.609	63.453	1.00	0.00	H
ATOM	4140	1HB	GLU	303	118.319	72.218	63.562	1.00	0.00	H
ATOM	4141	2HB	GLU	303	116.662	72.789	63.449	1.00	0.00	H
ATOM	4142	1HG	GLU	303	117.397	71.974	61.259	1.00	0.00	H
ATOM	4143	2HG	GLU	303	117.126	73.698	61.122	1.00	0.00	H
ATOM	4144	N	PHE	304	116.123	75.957	63.930	1.00	0.00	N
ATOM	4145	CA	PHE	304	115.408	77.255	63.706	1.00	0.00	C
ATOM	4146	C	PHE	304	116.187	78.601	64.004	1.00	0.00	C
ATOM	4147	O	PHE	304	115.678	79.671	63.666	1.00	0.00	O
ATOM	4148	CB	PHE	304	114.086	77.155	64.532	1.00	0.00	C
ATOM	4149	CG	PHE	304	112.952	78.103	64.094	1.00	0.00	C
ATOM	4150	CD1	PHE	304	112.209	77.828	62.941	1.00	0.00	C
ATOM	4151	CE1	PHE	304	111.199	78.696	62.531	1.00	0.00	C
ATOM	4152	CZ	PHE	304	110.911	79.832	63.280	1.00	0.00	C
ATOM	4153	CE2	PHE	304	111.637	80.110	64.436	1.00	0.00	C
ATOM	4154	CD2	PHE	304	112.654	79.248	64.842	1.00	0.00	C
ATOM	4155	H	PHE	304	115.943	75.378	64.761	1.00	0.00	H
ATOM	4156	HA	PHE	304	115.142	77.303	62.631	1.00	0.00	H
ATOM	4157	1HB	PHE	304	113.671	76.131	64.512	1.00	0.00	H
ATOM	4158	2HB	PHE	304	114.322	77.303	65.605	1.00	0.00	H
ATOM	4159	HD1	PHE	304	112.421	76.945	62.353	1.00	0.00	H
ATOM	4160	HE1	PHE	304	110.639	78.489	61.632	1.00	0.00	H
ATOM	4161	HZ	PHE	304	110.124	80.503	62.962	1.00	0.00	H
ATOM	4162	HE2	PHE	304	111.414	80.993	65.017	1.00	0.00	H
ATOM	4163	HD2	PHE	304	113.223	79.482	65.731	1.00	0.00	H
ATOM	4164	N	PHE	305	117.381	78.573	64.630	1.00	0.00	N
ATOM	4165	CA	PHE	305	118.152	79.787	65.016	1.00	0.00	C
ATOM	4166	C	PHE	305	119.662	79.644	64.585	1.00	0.00	C
ATOM	4167	O	PHE	305	120.540	79.402	65.413	1.00	0.00	O
ATOM	4168	CB	PHE	305	117.850	80.000	66.535	1.00	0.00	C
ATOM	4169	CG	PHE	305	118.007	81.423	67.096	1.00	0.00	C
ATOM	4170	CD1	PHE	305	117.364	82.517	66.501	1.00	0.00	C
ATOM	4171	CE1	PHE	305	117.504	83.793	67.039	1.00	0.00	C
ATOM	4172	CZ	PHE	305	118.254	83.979	68.198	1.00	0.00	C
ATOM	4173	CE2	PHE	305	118.865	82.894	68.816	1.00	0.00	C
ATOM	4174	CD2	PHE	305	118.748	81.623	68.264	1.00	0.00	C
ATOM	4175	H	PHE	305	117.712	77.629	64.875	1.00	0.00	H
ATOM	4176	HA	PHE	305	117.765	80.671	64.481	1.00	0.00	H
ATOM	4177	1HB	PHE	305	116.802	79.722	66.766	1.00	0.00	H
ATOM	4178	2HB	PHE	305	118.447	79.271	67.120	1.00	0.00	H
ATOM	4179	HD1	PHE	305	116.765	82.390	65.609	1.00	0.00	H
ATOM	4180	HE1	PHE	305	117.030	84.635	66.552	1.00	0.00	H
ATOM	4181	HZ	PHE	305	118.367	84.968	68.618	1.00	0.00	H
ATOM	4182	HE2	PHE	305	119.442	83.036	69.715	1.00	0.00	H
ATOM	4183	HD2	PHE	305	119.245	80.795	68.747	1.00	0.00	H
ATOM	4184	N	THR	306	119.955	79.784	63.270	1.00	0.00	N
ATOM	4185	CA	THR	306	121.282	79.388	62.661	1.00	0.00	C
ATOM	4186	C	THR	306	122.021	80.408	61.698	1.00	0.00	C
ATOM	4187	O	THR	306	123.248	80.336	61.626	1.00	0.00	O
ATOM	4188	CB	THR	306	121.171	77.981	61.978	1.00	0.00	C
ATOM	4189	OG1	THR	306	120.041	77.881	61.114	1.00	0.00	O
ATOM	4190	CG2	THR	306	121.072	76.801	62.954	1.00	0.00	C
ATOM	4191	H	THR	306	119.106	79.752	62.694	1.00	0.00	H
ATOM	4192	HA	THR	306	122.024	79.272	63.477	1.00	0.00	H
ATOM	4193	HB	THR	306	122.083	77.809	61.368	1.00	0.00	H
ATOM	4194	HG1	THR	306	119.374	77.379	61.601	1.00	0.00	H
ATOM	4195	1HG2	THR	306	121.035	75.832	62.425	1.00	0.00	H
ATOM	4196	2HG2	THR	306	121.942	76.765	63.637	1.00	0.00	H
ATOM	4197	3HG2	THR	306	120.171	76.867	63.591	1.00	0.00	H
ATOM	4198	N	SER	307	121.351	81.322	60.959	1.00	0.00	N
ATOM	4199	CA	SER	307	122.008	82.279	60.005	1.00	0.00	C
ATOM	4200	C	SER	307	121.336	83.709	59.965	1.00	0.00	C
ATOM	4201	O	SER	307	120.332	83.893	59.268	1.00	0.00	O
ATOM	4202	CB	SER	307	122.038	81.621	58.598	1.00	0.00	C
ATOM	4203	OG	SER	307	120.733	81.519	58.018	1.00	0.00	O
ATOM	4204	H	SER	307	120.334	81.201	60.982	1.00	0.00	H
ATOM	4205	HA	SER	307	123.069	82.426	60.287	1.00	0.00	H
ATOM	4206	1HB	SER	307	122.689	82.210	57.925	1.00	0.00	H
ATOM	4207	2HB	SER	307	122.506	80.618	58.645	1.00	0.00	H
ATOM	4208	HG	SER	307	120.294	82.369	58.183	1.00	0.00	H
ATOM	4209	N	GLY	308	121.864	84.730	60.673	0.00	0.00	N
ATOM	4210	CA	GLY	308	121.237	86.094	60.694	0.00	0.00	C
ATOM	4211	C	GLY	308	121.856	87.165	61.631	0.00	0.00	C

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ATOM   4212  OC  GLY   308     121.218  87.503  62.866  1.00  0.00           O
ATOM   4213  O   GLY   308     122.904  87.719  61.299  0.00  0.00           O
ATOM   4214  HC  GLY   308     120.660  86.703  63.195  1.00  0.00           H
ATOM   4215  H   GLY   308     122.592  84.429  61.338  1.00  0.00           H
ATOM   4216 1HA  GLY   308     121.270  86.515  59.672  0.00  0.00           H
ATOM   4217 2HA  GLY   308     120.155  86.006  60.912  0.00  0.00           H
TER
ATOM   4218  PG  ATP   400H     94.957  91.733  84.664  1.00 56.62           P
ATOM   4219  O1G ATP   400H     94.187  90.944  83.509  1.00 61.42           O
ATOM   4220  PB  ATP   400H     95.915  93.870  83.671  1.00 53.17           P
ATOM   4221  O1B ATP   400H     96.089  93.010  82.330  1.00 54.96           O
ATOM   4222  O1A ATP   400H     96.187  97.690  82.708  1.00 34.47           O
ATOM   4223  PA  ATP   400H     96.566  96.129  82.542  1.00 45.52           P
ATOM   4224  O5  ATP   400H     98.142  95.970  82.935  1.00 43.48           O
ATOM   4225  O3B ATP   400H     94.875  93.256  84.560  1.00 53.99           O
ATOM   4226  O2G ATP   400H     96.437  91.126  84.983  1.00 57.35           O
ATOM   4227  O3G ATP   400H     94.312  91.481  86.097  1.00 57.62           O
ATOM   4228  O2A ATP   400H     96.428  95.839  80.960  1.00 42.48           O
ATOM   4229  O3A ATP   400H     95.542  95.326  83.388  1.00 50.69           O
ATOM   4230  O2B ATP   400H     97.232  93.930  84.606  1.00 58.07           O
ATOM   4231  C5A ATP   400H     99.030  97.140  83.056  1.00 39.42           C
ATOM   4232  C5  ATP   400H    105.482  98.998  81.874  1.00 22.15           C
ATOM   4233  O2  ATP   400H    102.885  98.017  86.127  1.00 41.77           O
ATOM   4234  C2A ATP   400H    102.084  98.131  84.952  1.00 38.93           C
ATOM   4235  C2  ATP   400H    103.750 100.569  80.504  1.00 24.73           C
ATOM   4236  O4  ATP   400H    101.513  97.285  82.879  1.00 32.13           O
ATOM   4237  C1  ATP   400H    102.647  97.361  83.759  1.00 30.56           C
ATOM   4238  N9  ATP   400H    103.870  98.006  83.189  1.00 23.28           N
ATOM   4239  C8  ATP   400H    105.187  97.588  83.362  1.00 19.33           C
ATOM   4240  N7  ATP   400H    106.229  98.104  82.631  1.00 24.44           N
ATOM   4241  C4  ATP   400H    104.058  98.982  82.211  1.00 23.86           C
ATOM   4242  C6  ATP   400H    105.895  99.858  80.790  1.00 20.25           C
ATOM   4243  N6  ATP   400H    107.148  99.906  80.376  1.00 24.16           N
ATOM   4244  N1  ATP   400H    105.019 100.612  80.163  1.00 22.35           N
ATOM   4245  N3  ATP   400H    103.170  99.872  81.450  1.00 25.23           N
ATOM   4246  O3  ATP   400H    100.578  96.609  86.178  1.00 49.35           O
ATOM   4247  C3  ATP   400H    100.670  97.532  85.088  1.00 39.09           C
ATOM   4248  C4A ATP   400H    100.405  96.839  83.718  1.00 36.99           C
ATOM   4249 2H5  ATP   400H     99.210  97.562  82.051  1.00  0.00           H
ATOM   4250 1H5  ATP   400H     98.505  97.953  83.587  1.00  0.00           H
ATOM   4251  H2A ATP   400H    102.013  99.195  84.663  1.00  0.00           H
ATOM   4252  H2  ATP   400H    103.102 101.207  79.921  1.00  0.00           H
ATOM   4253  H1  ATP   400H    102.912  96.326  84.052  1.00  0.00           H
ATOM   4254  H8  ATP   400H    105.406  96.787  84.057  1.00  0.00           H
ATOM   4255 1H6  ATP   400H    107.816  99.359  80.926  1.00  0.00           H
ATOM   4256 2H6  ATP   400H    107.380 100.761  79.847  1.00  0.00           H
ATOM   4257  HO2 ATP   400H    103.375  97.170  86.050  1.00  0.00           H
ATOM   4258  HO3 ATP   400H    101.361  96.023  86.141  1.00  0.00           H
ATOM   4259  H3  ATP   400H     99.958  98.359  85.265  1.00  0.00           H
ATOM   4260  H4  ATP   400H    100.487  95.738  83.832  1.00  0.00           H
END
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Table 3. Inhibition of PLK1 enzymatic activity by adenosine, thioadenosines, and various thiol-reactive compounds in the presence or absence of dithiothreitol (+DTT or –DTT); IC_{50}; concentration with half-maximal inhibition.

Compound	IC_{50} (μM)	
	+ DTT	*- DTT*
Thimerosal	> 200	22
N-ethylmaleimide	> 200	55
Iodoacetamide	> 200	83
Adenosine	> 200	> 200
2'-Thioadenosine	> 200	120
5'-Thioadenosine	> 200	39

Table 4. PLK1 contact model (Maestro) for ATP.

PLK1		ATP atom	Distance (Å)	Contact cut-off ratio
Residue	*Atom*			
K178	NZ	O1B	3.1	1.0
K178	CE	O1B	4.0	1.2
R135	NH1	O1A	3.9	1.2
K61	CA	O1A	4.2	1.3
K61	N	O1A	3.0	1.0
G60	N	O1A	4.1	1.3
G60	C	O1A	3.2	1.0
R135	NH1	PA	3.3	1.0
R135	CZ	PA	4.3	1.2
G60	3HD2	PA	4.4	1.3
R135	NH1	O5	3.1	1.0
G63	N	O3G	3.9	1.2
R135	NE	O2A	3.9	1.2
F135	NH2	O2A	3.3	1.0
R136	CZ	O2A	3.0	0.9
F136	NH1	C5A	3.3	1.0
C67	SG	C5A	3.7	1.1
F183	CE2	C5	4.0	1.1
F183	CZ	C5	3.8	1.1
F183	CE1	C5	3.6	1.0
F183	CD1	C5	3.7	1.1
A80	CB	C5	4.2	1.2
F183	CD2	C5	4.2	1.2
F183	CG	C5	4.1	1.2
D194	OD1	O2	3.1	1.0

D194	CG	O2	3.2	1.0
K82	NZ	O2	3.4	1.1
K82	CE	O2	3.3	1.0
K82	CD	O2	3.3	1.0
K82	CG	O2	4.1	1.3
K82	CB	O2	3.9	1.2
C67	SG	C2A	4.1	1.2
D194	OD2	C2A	3.4	1.1
D194	OD1	C2A	3.6	1.1
D194	CG	C2A	3.8	1.1
K82	CD	C2A	4.4	1.3
C67	CB	C2A	3.9	1.1
F183	CZ	C2	4.6	1.3
F183	CE1	C2	3.7	1.0
F183	CD1	C2	3.9	1.1
C133	O	C2	3.4	1.0
C133	C	C2	4.4	1.3
A80	CB	C2	3.4	1.0
L59	CD1	C2	4.3	1.2
L59	CG	C2	4.4	1.3
C67	SG	O4	4.2	1.3
F183	CZ	O4	3.6	1.1
F183	CE1	O4	4.0	1.2
D194	CB	C1	4.4	1.3
F183	CZ	C1	3.8	1.1
F183	CE1	C1	4.4	1.3
D194	OD2	C1	3.3	1.0
D194	OD1	C1	3.8	1.1
D194	CG	C1	3.6	1.0
F183	CE2	N9	4.0	1.2
F183	CZ	N9	3.5	1.0
F183	CE1	N9	3.8	1.2
D194	OD2	N9	3.7	1.2
D194	CG	N9	4.3	1.3
D194	CB	C8	4.5	1.3
F183	CE2	C8	3.7	1.1
F183	CZ	C8	3.7	1.0
F183	CE1	C8	4.2	1.2
D194	OD2	C8	3.4	1.0
D194	CG	C8	4.1	1.2
G193	C	C8	4.1	1.2
G193	C	C8	4.3	1.2
D194	N	C8	3.9	1.2
F183	CD2	C8	4.4	1.2
L130	CD1	C8	3.9	1.1
F183	CE2	N7	3.8	1.1

F183	CZ	N7	3.9	1.1
F183	CE1	N7	4.2	1.2
F183	CD1	N7	4.4	1.3
G193	C	N7	4.4	1.3
G193	C	N7	4.0	1.2
F183	CD2	N7	4.0	1.2
F183	CG	N7	4.3	1.3
V114	CG2	N7	4.1	1.2
V114	CG1	N7	4.2	1.2
L130	CD1	N7	3.7	1.1
L130	CB	N7	4.4	1.3
F183	CE2	C4	4.2	1.2
F183	CZ	C4	3.5	1.0
F183	CE1	C4	3.4	1.0
F183	CD1	C4	4.0	1.1
A80	CB	C4	4.3	1.2
F183	CZ	C6	4.4	1.3
F183	CE1	C6	3.8	1.1
F183	CD1	C6	3.5	1.0
C133	O	C6	4.1	1.2
A80	CB	C6	3.7	1.1
F183	CD2	C6	4.5	1.3
F183	CG	C6	3.9	1.1
V114	CG1	C6	4.4	1.3
C133	CB	C6	4.5	1.3
C133	N	C6	4.1	1.2
E131	O	C6	3.4	1.0
F183	CD1	N6	4.0	1.2
F183	CG	N6	4.0	1.2
V114	CG2	N6	3.8	1.1
V114	CG1	N6	3.4	1.0
V114	CB	N6	4.3	1.3
C133	SG	N6	4.4	1.3
C133	CB	N6	3.7	1.1
C133	CA	N6	4.2	1.3
C133	N	N6	3.8	1.2
E131	O	N6	2.8	0.9
E131	C	N6	4.0	1.2
F183	CE1	N1	3.9	1.1
F183	CD1	N1	3.6	1.1
C133	O	N1	3.1	1.0
C133	C	N1	3.9	1.1
F183	CD1	N1	3.3	1.0
F183	CG	N1	4.4	1.3
C133	CB	N1	4.3	1.3
C133	CA	N1	4.0	1.2

C133	N	N1	3.4	1.1
E131	O	N1	3.5	1.1
C67	SG	N3	4.5	1.3
F183	CZ	N3	4.1	1.2
F183	CE1	N3	3.5	1.0
F183	CD1	N3	4.1	1.2
F183	CD1	N3	3.9	1.1
L59	CD1	N3	4.1	1.2
D194	OD2	O3	3.9	1.3
D194	CG	O3	3.5	1.1
K82	CD	O3	4.1	1.3
C67	SG	C3	3.8	1.1
D194	OD1	C3	3.6	1.1
D194	CG	C3	4.1	1.2
C67	CB	C3	4.1	1.2
C67	SG	C4A	4.1	1.2
D194	OD1	C4A	4.1	1.2

Table 5. PLK1 contact model (Quanta) for ATP.

PLK1 residue	**Residue atom**	**Protein – ligand atom distance (Å)**
L59	HG	3.5
L59	HD11	3.2
L59	HG	2.6
L59	HD13	3.1
G60	CA	2.8
G60	C	3.2
G60	HA1	1.9
G60	HA2	3.1
G60	HA1	3.5
G60	HA1	3.5
G60	HA1	2.9
K61	N	3.0
K61	H	2.2
G62	HA1	3.1
G63	H	2.9
C67	HG	3.1
C67	HB2	3.0
C67	HG	3.2
C67	HG	3.0
C67	HG	3.4
C67	HB2	3.3
C67	HG	3.2
C67	HG	3.2

C67	HG	2.9
C67	SG	3.0
C67	HG	2.7
C67	CB	2.9
C67	SG	3.3
C67	HB1	2.9
C67	HB2	2.2
C67	HG	2.5
C67	CB	3.3
C67	SG	3.0
C67	HB2	2.6
C67	HG	2.7
A80	CB	3.4
A80	HB1	2.9
A80	HB2	3.1
A80	HB3	3.2
A80	CB	3.3
A80	HB1	3.2
A80	HB2	2.9
A80	HB3	3.1
A80	HB1	3.0
A80	HB1	3.2
A80	HB2	3.0
A80	HB3	3.4
K82	CD	3.3
K82	CE	3.3
K82	NZ	3.4
K82	HZ2	2.8
K82	HB2	3.1
K82	HD1	2.4
K82	HE2	3.0
K82	HD1	3.4
K82	HD1	3.1
K82	HB2	3.5
K82	CE	3.4
K82	NZ	3.1
K82	HZ1	3.5
K82	HZ2	2.2
K82	HD1	2.9
K82	HE2	3.1
K82	HZ2	3.2
K82	HD1	3.2
V114	HG13	3.2
V114	HG23	3.1
V114	CG1	3.4
V114	HG12	3.1

V114	HG13	2.7
V114	HG21	3.4
V114	HG23	3.2
V114	CB	3.3
V114	CG1	2.5
V114	CG2	2.9
V114	HG11	3.4
V114	HG12	2.5
V114	HG13	1.8
V114	HG21	2.8
V114	HG23	2.3
V114	HG12	3.2
V114	HG13	3.2
L130	HD11	3.1
L130	HD11	2.8
L130	HD11	3.0
L130	HB2	3.2
E131	O	3.4
E131	O	2.8
E131	O	3.5
E131	O	3.3
E131	C	3.1
E131	O	2.0
C133	O	3.4
C133	H	3.3
C133	H	2.9
C133	HB1	2.7
C133	N	3.4
C133	O	3.1
C133	H	2.8
C133	O	3.0
C133	HB1	3.4
C133	N	2.9
C133	CB	3.1
C133	H	2.0
C133	HB1	2.3
R135	HH12	3.0
R135	NH1	3.3
R135	HH12	2.7
R135	HH11	2.9
R135	NH1	3.1
R135	HH12	2.9
R135	HH11	2.7
R135	CZ	3.0
R135	NH1	2.3
R135	NH2	3.3

R135	HH12	1.9
R135	HH11	2.1
R135	HH22	2.8
R135	NH1	3.3
R135	HH12	3.0
R135	HH11	3.4
R135	NH1	2.6
R135	HH12	2.3
R135	HH11	3.0
K178	NZ	3.1
K178	HZ1	3.1
K178	HZ2	2.3
F183	HE1	3.3
F183	HZ	2.8
F183	HZ	3.2
F183	CZ	3.5
F183	HZ	3.2
F183	CE1	3.4
F183	HE1	3.3
F183	HD1	3.3
F183	CE1	3.5
F183	HE1	3.0
F183	HZ	3.1
G193	HA2	3.5
G193	HA2	3.1
G193	C	3.4
G193	HA2	3.2
D194	CG	3.2
D194	OD1	3.1
D194	OD2	2.5
D194	OD2	3.4
D194	OD2	3.3
D194	OD2	3.4
D194	OD1	2.6
D194	CB	3.3
D194	CG	2.6
D194	OD1	3.0
D194	OD2	2.7
D194	HB2	2.8
D194	N	2.9
D194	CG	3.3
D194	OD2	2.5
D194	H	2.7
D194	HB2	3.4
D194	CG	2.2
D194	OD1	2.4

D194	OD2	1.6
D194	CG	2.6
D194	OD1	1.7
D194	OD2	3.1

Table 6. PLK1 contact model (Maestro) for 5'-thioadenosine.

PLK1		**5'-Thio-adenosine atom**	**Distance (Å)**	**Contact cut-off ratio**
Residue	*Atom*			
G60	CA	S5	4.0	1.1
C67	N	S5	3.3	1.0
K66	C	S5	3.9	1.1
K66	CA	S5	4.1	1.2
K61	CA	S5	4.3	1.2
K61	N	S5	3.9	1.2
G60	O	S5	3.4	1.0
G60	C	S5	3.5	1.0
C67	SG	S5	3.3	0.9
C67	CB	S5	3.6	1.0
C67	CA	S5	4.1	1.2
R135	NH2	C5A	3.7	1.2
R135	CZ	C5A	4.0	1.2
R135	NH2	C5A	3.6	1.1
C67	SG	C5A	3.6	1.0
C67	CB	C5A	4.2	1.2
F183	CZ	C5	3.5	1.0
F183	CE1	C5	3.5	1.0
F183	CD1	C5	4.1	1.2
A80	CB	C5	3.8	1.1
F183	CE2	C5	4.0	1.2
D194	OD1	O2	3.6	1.2
D194	CG	O2	3.3	1.0
K82	NZ	O2	3.1	1.0
K82	CB	O2	3.8	1.2
K82	CE	O2	3.1	1.0
K82	CD1	O2	3.2	1.0
K82	CG	O2	4.0	1.3
D194	OD2	C2A	3.4	1.0
D194	OD1	C2A	3.6	1.1
D194	CG	C2A	3.8	1.1
K82	CB	C2A	4.1	1.2
C67	CB	C2A	3.9	1.2
K82	CE	C2A	4.2	1.2
K82	CD	C2A	3.9	1.1
F183	CZ	C2	4.2	1.2

C133	O	C2	3.5	1.1
F183	CE1	C2	3.5	1.0
F183	CD1	C2	4.0	1.2
R135	NH2	C2	4.1	1.3
L59	CD1	C2	3.8	1.1
L59	CG	C2	4.2	1.2
A80	CB	C2	3.4	1.0
R135	NH2	O4	3.0	1.0
R135	CZ	O4	3.3	1.0
D194	OD1	O4	3.8	1.3
R135	NH2	O4	2.8	0.9
C67	SG	O4	3.6	1.1
C67	CB	O4	3.9	1.2
F183	CZ	C1	4.2	1.2
R135	NH2	C1	3.7	1.2
R135	CZ	C1	4.3	1.3
D194	OD2	C1	3.6	1.1
D194	OD1	C1	3.3	1.0
D194	CG	C1	3.7	1.1
R135	NH2	C1	3.9	1.2
C67	CB	C1	4.4	1.3
F183	CZ	N9	3.7	1.1
F183	CE1	N9	4.2	1.3
F183	CZ	C8	3.8	1.1
D194	OD2	C8	4.3	1.2
F183	CE2	C8	4.1	1.2
L130	CD1	C8	3.6	1.1
F183	CZ	N7	3.8	1.1
F183	CE1	N7	4.2	1.3
F183	CE2	N7	3.9	1.2
L130	CD1	N7	3.6	1.1
L130	CB	N7	3.9	1.2
F183	CZ	C4	3.5	1.0
F183	CE1	C4	3.6	1.0
R135	NH2	C4	4.1	1.2
A80	CB	C4	4.0	1.2
F183	CE2	C4	4.4	1.3
F183	CZ	C6	3.9	1.1
C133	O	C6	4.1	1.3
F183	CE1	C6	3.4	1.0
F183	CD1	C6	3.5	1.0
A80	CB	C6	3.5	1.0
F183	CD2	C6	4.5	1.3
F183	CE2	C6	4.4	1.3
F183	CG	C6	4.1	1.2
C133	N	C6	4.1	1.3

E131	O	C6	3.5	1.1
F183	CE1	N6	4.0	1.2
F183	CD1	N6	3.7	1.1
A80	CB	N6	4.1	1.3
F183	CG	N6	3.9	1.2
C133	SG	N6	4.3	1.3
C133	SB	N6	3.6	1.1
F183	CE1	N6	4.1	1.3
C133	N	N6	3.7	1.2
E131	O	N6	2.9	1.0
V114	CG2	N6	4.1	1.3
V114	CG1	N6	3.7	1.1
F125	CE2	N6	4.0	1.2
F183	CZ	N1	4.3	1.3
C133	O	N1	3.1	1.0
C133	C	N1	3.8	1.2
F183	CE1	N1	3.4	1.0
F183	CD1	N1	3.6	1.1
A80	CB	N1	3.3	1.0
C133	CA	N1	4.1	1.2
C133	N	N1	3.6	1.1
E131	O	N1	3.8	1.2
F183	CZ	N3	4.0	1.2
F183	CE1	N3	3.6	1.1
R135	NH2	N3	3.4	1.1
C67	SG	N3	4.0	1.2
L59	CD1	N3	3.8	1.2
A80	CB	N3	3.8	1.1
D194	OD2	O3	3.0	0.9
D194	CG	O3	3.2	1.0
K82	NZ	O3	3.7	1.2
K82	CE	O3	4.1	1.3
K82	CD	O3	3.5	1.1
D194	OD2	C3	3.7	1.1
D194	OD1	C3	3.3	1.0
D194	CG	C3	3.9	1.2
C67	SG	C3	4.5	1.3
C67	CB	C3	4.1	1.2
K82	CD	C3	3.8	1.1
R135	NH2	C4A	3.4	1.0
R135	CZ	C4A	3.9	1.1
D194	OD2	C4A	4.4	1.3
D194	OD1	C4A	3.3	1.0
D194	CG	C4A	4.2	1.2
R135	NH2	C4A	3.6	1.1
C67	SG	C4A	4.0	1.1

C67	CB	C4A	4.2	1.2

Table 7. PLK1 contact model (Quanta) for 5'-thioadenosine.

PLK1 residue	Residue atom	Protein – ligand atom distance (Å)
L59	HG	3.4
L59	HD11	3.5
L59	HD13	3.3
L59	HD11	3.2
L59	CG	3.2
L59	CD1	3.0
L59	HG	2.5
L59	HD11	2.9
L59	HD13	2.5
G60	C	3.2
G60	O	3.2
G60	HA1	3.1
G60	HA1	3.3
C67	N	3.1
C67	CB	3.1
C67	SG	2.0
C67	H	2.7
C67	HB2	3.0
C67	SG	3.2
C67	HB2	3.0
C67	SG	3.4
C67	HB2	3.4
C67	HB2	3.1
C67	SG	3.4
C67	CB	3.1
C67	HB1	3.2
C67	HB2	2.1
C67	CB	3.5
C67	HB2	2.6
A80	HB1	3.4
A80	HB3	3.2
A80	CB	3.4
A80	HB1	2.8
A80	HB2	3.1
A80	HB1	3.2
A80	CB	3.5
A80	HB1	3.3
A80	HB2	3.4
A80	HB3	3.0

A80	HB3	3.4
A80	CB	3.3
A80	HB1	3.1
A80	HB2	2.9
A80	HB3	3.2
A80	HB1	2.9
A80	HB1	3.3
A80	HB2	3.3
K82	CD	3.2
K82	CE	3.1
K82	NZ	3.1
K82	HZ2	2.5
K82	HB2	3.0
K82	HD1	2.5
K82	HE2	2.6
K82	HB2	3.1
K82	HD1	2.9
K82	HZ2	3.1
K82	HD1	2.5
K82	HD1	2.7
K82	CB	3.5
K82	HB2	2.4
K82	HD1	3.1
K82	CE	3.3
K82	NZ	2.9
K82	HZ2	2.0
K82	HD1	2.9
K82	HE2	3.1
K82	HZ2	2.9
K82	HD1	3.2
K82	HB2	3.3
K82	HD1	2.6
V114	HG13	3.3
V114	HG13	2.9
V114	HG23	3.5
V114	CG1	2.8
V114	CG2	3.3
V114	HG12	2.8
V114	HG13	1.9
V114	HG21	3.2
V114	HG23	2.7
V114	HG13	3.5
L130	HD13	3.2
L130	HD11	3.0
L130	HB1	3.4
L130	HB2	3.4

L130	HD13	3.5
L130	HD11	2.8
L130	CD1	3.2
L130	HD13	2.9
L130	HD11	2.6
L130	HB2	3.2
E131	O	3.5
E131	O	2.9
E131	O	3.2
E131	O	2.5
C133	H	3.2
C133	H	2.9
C133	HB1	2.7
C133	O	3.1
C133	H	2.7
C133	O	3.1
C133	HB1	3.2
C133	N	2.7
C133	CA	3.2
C133	CB	2.8
C133	SG	3.4
C133	H	2.0
C133	HB1	2.0
R135	HH11	3.1
R135	HH22	3.2
R135	CZ	3.3
R135	NH1	2.8
R135	NH2	3.0
R135	HH11	1.8
R135	HH22	2.1
R135	HH11	3.0
R135	HH22	2.7
R135	HH11	3.4
R135	HH11	3.3
R135	NH1	3.4
R135	HH11	2.8
R135	NH2	3.4
R135	HH11	2.8
R135	HH22	2.5
R135	CZ	3.1
R135	NH1	2.8
R135	NH2	3.1
R135	HH12	3.5
R135	HH11	2.6
R135	HH22	2.9
R135	NH2	3.4

R135	HH11	3.4
R135	HH22	2.5
R135	NH2	2.9
R135	HH11	3.2
R135	HH21	3.5
R135	HH22	2.1
F183	CE1	3.5
F183	HE1	2.9
F183	HZ	3.3
F183	HZ	3.1
F183	HZ	3.5
F183	HE1	3.4
F183	HZ	3.2
F183	CE1	3.4
F183	CE1	3.4
F183	HD1	3.4
F183	HE1	3.2
F183	HE1	2.9
F183	HE1	3.2
F183	HZ	2.9
D194	CG	3.3
D194	OD2	2.5
D194	OD2	3.4
D194	OD1	3.3
D194	CG	3.2
D194	OD1	2.6
D194	OD2	3.0
D194	OD1	3.3
D194	OD1	3.3
D194	CG	2.7
D194	OD1	2.4
D194	OD2	2.9
D194	OD2	3.4
D194	H	3.3
D194	CG	2.4
D194	OD1	2.8
D194	OD2	1.5
D194	CG	2.3
D194	OD1	1.7
D194	OD2	2.3
D194	OD1	2.4

Table 8. PLK1 contact model (Maestro) for staurosporine.

PLK1		Staurosporine atom	Distance (Å)	Contact cut-off ratio
Residue	*Atom*			
C67	CB	O4	3.5	1.1
D194	OD2	C21	4.1	1.2
C67	CB	C23	4.2	1.2
C67	SG	C18	3.7	1.0
C67	CB	C18	3.9	1.1
C67	SG	C19	4.3	1.2
C67	CB	C19	4.2	1.2
D194	OD1	C16	3.4	1.0
D194	CG	C16	4.0	1.2
G193	O	C16	3.7	1.1
G193	C	C16	4.3	1.3
L130	CD1	C16	4.3	1.3
F183	CE1	C14	3.3	1.0
F183	CZ	C14	3.7	1.1
F183	CD1	C14	4.1	1.2
L130	CD2	C14	4.3	1.3
L130	CD1	C14	3.9	1.1
L130	CG	C14	4.2	1.2
L130	CB	C14	3.8	1.1
A80	CB	C14	4.2	1.2
D194	OD1	C15	3.9	1.2
G193	O	C15	3.6	1.1
G193	C	C15	4.1	1.2
F183	CE1	C15	3.8	1.1
L130	CD2	C15	3.9	1.2
L130	CD1	C15	3.6	1.1
L130	CG	C15	4.1	1.2
L130	CB	C15	4.3	1.2
F183	CE1	C13	3.8	1.1
F183	CZ	C13	4.3	1.2
F183	CD1	C13	4.2	1.2
C67	SG	C13	4.6	1.3
A80	CB	C13	3.4	1.0
C67	SG	C12	3.8	1.1
A80	CB	C12	4.0	1.2
C67	SG	C17	4.0	1.1
C67	SG	N2	3.9	1.1
C67	CB	N2	4.0	1.2
R135	CG	C7	4.0	1.2
L59	CD1	C7	3.9	1.2
L59	CG	C7	4.3	1.3

L59	CB	C7	3.8	1.1
C67	SG	C10	4.1	1.2
A80	CB	C10	4.3	1.3
L59	CD1	C10	3.9	1.1
C67	SG	C11	3.6	1.0
C67	CB	C11	4.4	1.3
A80	CB	C11	4.4	1.3
R135	CG	C6	4.0	1.2
L59	C	C6	4.4	1.3
L59	CB	C6	3.8	1.1
G60	CA	N3	4.2	1.3
G60	CA	C20	3.8	1.1
G60	N	C20	4.2	1.3
L59	C	C20	4.3	1.2
L59	O	C20	4.1	1.3
R135	CG	C5	3.7	1.1
G60	CA	C5	4.3	1.3
G60	N	C5	4.2	1.3
L59	C	C5	3.9	1.1
L59	CB	C5	4.1	1.2
L59	O	C5	3.7	1.1
R135	CG	C4	3.5	1.0
R135	NE	C4	3.7	1.1
R135	CD	C4	4.0	1.2
L59	C	C4	3.8	1.1
L59	CB	C4	4.4	1.3
L59	O	C4	3.2	1.0
R135	CG	C3	4.1	1.2
R135	CD	C3	4.4	1.3
L59	C	C3	4.1	1.2
L59	O	C3	3.2	1.0
G60	CA	C2	4.1	1.2
L59	O	C2	3.8	1.2
G60	CA	C1	3.7	1.1
L59	O	C1	4.2	1.3
C67	CB	C25	4.4	1.3
G60	CA	C25	4.3	1.3
D194	OD2	C23	4.0	1.2
D194	CG	C22	4.0	1.2
D194	OD2	C22	3.5	1.0
D194	OD1	C26	3.9	1.2
D194	CG	C26	4.0	1.2
D194	OD2	C26	3.4	1.0
K82	CE	C26	4.2	1.2
K82	CD	C26	3.9	1.1
K82	CG	C26	4.4	1.3

C67	CB	C26	4.2	1.2
G180	O	O6	3.7	1.2
N181	O	C27	3.8	1.2
N181	C	C27	4.2	1.2
N181	CA	C27	3.8	1.1
G180	O	C27	3.6	1.1
G180	C	C27	4.2	1.2
D194	CG	C27	4.4	1.3
D194	N	C27	3.9	1.2
G193	O	C27	3.1	1.0
G193	C	C27	4.0	1.2
G180	O	N4	3.6	1.2
D194	OD2	N4	4.2	1.3
N181	OD1	C28	4.1	1.3
K178	NZ	C28	3.7	1.1
D176	OD2	C28	4.4	1.3
D194	CG	C28	4.1	1.2
D194	CB	C28	4.1	1.2
D194	OD2	C28	3.3	1.0
C133	O	C9	3.5	1.1
C133	C	C9	3.8	1.1
C133	N	C9	3.9	1.2
A80	CB	C9	3.9	1.2
L59	CD1	C9	3.9	1.1
R134	CA	N1	4.0	1.2
R134	N	N1	4.0	1.3
C133	O	N1	2.8	0.9
C133	C	N1	3.4	1.0
L59	CD2	N1	4.2	1.3
L59	CD1	N1	3.8	1.2
R135	CG	O5	3.8	1.2
R135	NH2	O5	3.1	1.0
R135	CZ	O5	3.4	1.1
R135	CD	O5	3.8	1.2
L59	CD2	O5	3.6	1.1
L59	CG	O5	4.1	1.3
L59	CB	O5	3.9	1.2
R135	CG	C8	3.9	1.1
C133	O	C8	3.8	1.2
R135	CZ	C8	4.4	1.3
R135	NE	C8	3.6	1.1
R135	CD	C8	4.3	1.3
L59	CD2	C8	3.9	1.1
L59	CD1	C8	3.8	1.1
L59	CG	C8	4.0	1.2
L59	CB	C8	3.9	1.1

Table 9. PLK1 contact model (Quanta) for staurosporine.

PLK1 residue	Residue atom	Protein – ligand atom distance (Å)
L59	HB1	2.8
L59	HD13	3.1
L59	HD13	3.0
L59	HB1	2.9
L59	HB1	3.2
L59	O	3.2
L59	HB1	3.4
L59	O	3.2
L59	HD13	2.8
L59	HD13	2.7
L59	HD22	3.3
L59	HB1	3.0
L59	HD22	2.6
L59	HB1	2.9
L59	HD13	2.9
L59	HD22	2.9
L59	O	3.4
L59	HB1	3.1
L59	O	3.5
L59	CD1	3.3
L59	HD13	2.4
L59	HD13	3.1
L59	HD22	3.2
G60	HA1	3.2
G60	HA1	2.8
G60	HA1	3.5
G60	HA1	3.3
G60	HA1	2.7
G60	HA1	3.3
G60	HA1	2.9
G60	CA	3.4
G60	C	3.4
G60	HA1	2.5
C67	HB1	2.8
C67	HB2	3.3
C67	HB1	3.3
C67	HB1	3.4
C67	HB1	3.1
C67	HB1	3.5
C67	CB	3.4

C67	HB1	2.3
C67	HG	3.5
A80	HB2	3.5
A80	CB	3.4
A80	HB2	3.0
A80	HB3	2.9
A80	HB3	3.1
A80	HB3	3.4
A80	HB1	3.3
A80	HB2	3.4
A80	CB	3.0
A80	HB1	3.0
A80	HB2	2.6
A80	HB3	2.7
A80	CB	2.9
A80	HB1	2.2
A80	HB2	3.3
A80	HB3	2.7
K82	HD2	3.0
K82	HD2	3.4
K82	HD2	3.3
K82	HE1	3.1
K82	CD	3.5
K82	HZ3	2.9
K82	HD2	2.5
K82	HE1	3.3
K82	HB2	3.1
K82	HG1	3.3
K82	HD2	2.7
L130	HD12	3.3
L130	HB1	3.0
L130	HD12	2.9
L130	HD22	3.5
L130	HD12	2.6
L130	HD22	3.1
L130	CD1	3.4
L130	CD2	3.1
L130	HD12	2.6
L130	HD22	2.2
L130	HD21	3.4
L130	CB	3.1
L130	HB1	2.4
L130	HB2	2.8
L130	HD12	3.1
L130	HD22	3.1
E131	O	3.4

L132	HA	3.5
L132	C	3.4
C133	O	2.8
C133	C	3.4
C133	O	3.5
C133	H	3.4
C133	HB1	3.1
C133	N	3.5
C133	H	3.4
C133	C	2.7
C133	O	1.8
C133	O	1.8
R134	HA	3.1
R134	HA	3.4
R134	HA	3.4
R134	HA	2.8
R135	HG2	3.0
R135	HG2	3.3
R135	HG1	3.0
R135	HG2	3.3
R135	CG	3.5
R135	HE	3.2
R135	HG1	2.7
R135	HG2	3.3
R135	HG1	3.1
R135	HE	3.4
R135	NE	2.8
R135	CZ	3.4
R135	NH2	3.1
R135	HE	1.7
R135	HG2	3.0
R135	HH21	2.2
R135	HE	2.6
R135	HG2	2.9
R135	HH21	3.4
R135	CG	3.5
R135	NE	3.0
R135	HE	2.4
R135	HG1	3.0
R135	HG2	3.2
R135	HH21	3.2
R135	H	3.3
R135	HE	3.5
R135	HE	1.7
K178	HZ1	3.5
K178	HZ1	2.7

K178	HZ1	3.2
K178	NZ	3.5
K178	HZ1	2.5
K178	NZ	2.9
K178	HZ1	2.0
K178	HZ2	3.2
K178	HZ3	3.5
K178	HZ1	2.0
G180	O	3.5
G180	O	3.3
G180	O	2.6
N181	HA	2.8
N181	CA	3.4
N181	OD1	3.2
N181	HA	2.3
N181	CA	3.2
N181	C	3.5
N181	O	3.2
N181	HA	2.3
N181	OD1	3.2
F183	CE1	3.3
F183	HE1	2.8
F183	HE1	2.9
F183	HE1	2.9
F183	CE1	3.0
F183	CZ	3.0
F183	HE1	2.6
F183	HZ	2.7
G193	O	3.1
G193	HA2	3.4
G193	O	3.0
G193	O	3.3
G193	O	2.5
D194	OD1	3.4
D194	OD2	3.4
D194	H	3.0
D194	OD2	3.3
D194	HB2	3.3
D194	CG	3.0
D194	OD1	2.4
D194	OD2	3.5
D194	CG	2.9
D194	OD1	3.4
D194	OD2	2.5
D194	HB2	3.2
D194	OD2	3.3

D194	CG	3.0
D194	OD1	2.8
D194	OD2	2.6
D194	N	3.2
D194	H	2.2
D194	HB2	2.8
D194	H	3.5
D194	H	3.0
D194	OD2	2.7
D194	CB	3.2
D194	CG	3.3
D194	OD2	2.9
D194	HB1	3.5
D194	HB2	2.3
D194	H	2.2

Table 10. PLK1 contact model (Maestro) for 4-[4-(4-methyl-2-methylamino-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol.

PLK1		**Ligand atom**	**Distance (Å)**	**Contact cut-off ratio**
Residue	*Atom*			
D194	OD2	NM1	3.8	1.2
K82	CD	NM1	4.1	1.3
D194	CG	CM12	4.0	1.2
D194	OD2	CM12	3.6	1.1
F64	CG	CM12	4.0	1.2
D194	OD1	CM12	3.5	1.1
K82	NZ	CM12	4.2	1.3
K82	CD	CM12	3.9	1.1
F64	CD1	CM12	4.1	1.2
F64	CB	CM12	3.8	1.1
D194	CG	C	4.0	1.2
D194	OD2	C	3.5	1.0
D194	OD1	C	3.8	1.2
K82	CD	C	4.1	1.2
C67	CB	C	4.0	1.2
D194	CG	N	3.5	1.1
D194	OD2	N	3.4	1.0
D194	OD1	N	3.1	1.0
K82	NZ	N	3.4	1.1
K82	CE	N	3.4	1.0
K82	CD	N	3.5	1.1
K82	CB	N	4.2	1.3
D194	CG	C1	3.9	1.1

D194	OD2	C1	3.8	1.1
D194	OD1	C1	3.7	1.2
K82	NZ	C1	4.1	1.2
K82	CE	C1	4.1	1.2
L130	CD1	C1	4.1	1.2
D194	CG	CM2	3.7	1.1
D194	CB	CM2	4.3	1.3
D194	CA	CM2	4.1	1.2
D194	OD2	CM2	4.0	1.2
D194	NZ	CM2	3.6	1.1
D194	OD1	CM2	3.5	1.1
K82	NZ	CM2	3.9	1.2
K82	CE	CM2	4.1	1.2
L130	CD2	CM2	3.9	1.2
L130	CD1	CM2	3.8	1.1
D194	OD2	S	4.2	1.2
C67	SG	S	3.5	1.0
C67	CB	S	3.3	0.9
D194	OD2	C2	4.3	1.3
F183	CZ	C2	4.1	1.2
C67	SG	C2	3.9	1.1
C67	CB	C2	4.3	1.3
F183	CZ	N1	4.0	1.2
F183	CG	N1	4.2	1.3
F183	CE1	N1	3.5	1.1
F183	CD1	N1	3.6	1.1
C133	N	N1	3.8	1.2
E131	O	N1	3.6	1.2
A80	CB	N1	3.3	1.0
C133	O	N1	3.4	1.1
C133	C	N1	4.2	1.3
F183	CD2	C3	4.3	1.3
F183	CE2	C3	4.2	1.2
F183	CZ	C3	4.0	1.2
F183	CG	C3	4.3	1.3
F183	CE1	C3	4.0	1.2
F183	CD1	C3	4.1	1.2
E131	O	C3	3.5	1.1
A80	CB	C3	3.5	1.0
F183	CE2	C4	4.0	1.2
F183	CZ	C4	3.8	1.1
F183	CE1	C4	4.2	1.2
L130	CD1	C4	4.1	1.2
L130	CB	C4	4.3	1.3
A80	CB	C4	3.9	1.2
F183	CE2	C5	4.2	1.2

F183	CZ	C5	3.6	1.0
F183	CE1	C5	4.0	1.2
C67	SG	C5	3.9	1.1
A80	CB	C5	4.1	1.2
F183	CZ	N6	3.6	1.1
F183	CE1	N6	3.5	1.1
C67	SG	N6	3.5	1.0
A80	CB	N6	3.9	1.2
F183	CZ	C7	3.8	1.1
F183	CE1	C7	3.3	1.0
F183	CD1	C7	3.8	1.1
C67	SG	C7	4.2	1.2
A80	CB	C7	3.5	1.0
C133	O	C7	3.6	1.1
F183	CE1	N2	3.4	1.0
F183	CD1	N2	3.8	1.2
A80	CB	N2	4.2	1.3
C133	O	N2	2.8	0.9
C133	C	N2	4.0	1.2
L59	CD2	N2	3.9	1.2
F183	CE1	C8	3.9	1.1
C133	O	C8	3.6	1.1
L59	CD2	C8	3.8	1.1
L59	CG	C8	4.2	1.2
L59	CB	C8	4.1	1.2
R135	CB	C9	4.4	1.3
R135	N	C9	4.1	1.3
R134	CA	C9	4.2	1.2
C133	O	C9	3.4	1.0
C133	C	C9	4.4	1.3
L59	CD2	C9	3.9	1.1
L59	CG	C9	4.0	1.2
L59	CB	C9	4.3	1.2
R135	NH2	O11	2.9	1.0
R135	NH1	O11	3.4	1.1
R135	CZ	O11	3.5	1.1
L59	C	O11	3.5	1.1
R135	NH2	C10	4.1	1.3
R135	CZ	C10	4.4	1.3
L59	CG	C10	4.1	1.2
L59	CB	C10	4.2	1.2
R135	NH2	C11	3.4	1.1
R135	NH1	C11	3.5	1.1
R135	CZ	C11	3.6	1.1
L59	C	C11	3.7	1.1
L59	CG	C11	4.4	1.3

L59	CB	C11	4.0	1.2
L59	O	C11	3.2	1.0
L59	CA	C11	4.3	1.2
R135	NH1	C12	4.2	1.3
F183	CE1	C12	4.3	1.2
C67	SG	C12	4.3	1.2
L59	C	C12	4.4	1.3
L59	CD2	C12	4.4	1.3
L59	CG	C12	4.4	1.3
L59	CB	C12	3.8	1.1
R135	NH2	C13	4.0	1.2
R135	NH1	C13	3.3	1.0
R135	CZ	C13	3.8	1.1
G60	CA	C13	4.3	1.2
G60	N	C13	3.8	1.2
L59	C	C13	3.5	1.0
L59	CB	C13	3.8	1.1
L59	O	C13	3.4	1.1
L59	CA	C13	4.2	1.2

Table 11. PLK1 contact model (Quanta) for 4-[4-(4-methyl-2-methylamino-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol.

PLK1 residue	Residue atom	Protein – ligand atom distance (Å)
L59	O	1.7
L59	HD23	2.9
L59	HB1	3.1
L59	HD23	2.9
L59	HB1	3.5
L59	HG	3.3
L59	HD23	3.2
L59	O	2.7
L59	HG	3.3
L59	O	3.2
L59	HB1	3.2
L59	HB1	2.7
L59	O	3.4
L59	HB1	2.8
L59	HD23	3.0
L59	HD23	3.3
L59	HG	3.5
L59	C	2.7
L59	O	1.7

L59	HA	3.4
L59	HB1	3.1
L59	C	3.2
L59	O	3.2
L59	HB1	3.1
G60	N	3.2
G60	CA	3.4
G60	HA1	2.6
F64	HB2	2.9
F64	HB2	3.5
F64	CB	3.4
F64	HB2	2.4
F64	HD1	3.2
F64	CB	3.2
F64	HB1	3.0
F64	HB2	2.5
C67	HB1	3.3
C67	HB1	3.0
C67	CB	3.3
C67	HB1	2.6
C67	HB2	3.4
C67	SG	3.5
C67	HB1	3.0
C67	HB2	3.3
A80	CB	3.3
A80	HB1	3.0
A80	HB2	3.1
A80	HB3	3.0
A80	CB	3.5
A80	HB1	3.3
A80	HB3	2.9
A80	HB1	3.4
A80	HB3	3.4
A80	HB1	3.3
A80	HB1	3.0
A80	HB1	2.9
A80	HB2	3.4
A80	HB3	3.0
K82	HD1	3.0
K82	HD1	2.9
K82	HD1	3.1
K82	CD	3.5
K82	CE	3.4
K82	NZ	3.4
K82	HZ2	2.7
K82	HB2	3.4

K82	HD1	2.7
K82	HE2	3.0
K82	HE2	3.3
K82	HZ2	3.4
K82	HE2	3.3
K82	HZ2	3.0
K82	HD1	3.4
K82	CD	3.0
K82	HZ2	3.2
K82	HD1	2.2
K82	HD2	2.9
K82	HE2	3.0
K82	NZ	3.1
K82	HZ2	2.6
K82	HZ3	2.9
K82	HE2	3.1
V114	HG12	2.9
V114	HG12	3.5
L130	HD13	3.3
L130	HD13	3.1
L130	HD22	3.2
L130	HB1	3.5
L130	HB1	3.3
L130	HD13	3.0
L130	HD22	3.1
L130	CG	3.4
L130	CD1	2.8
L130	CD2	2.9
L130	HD13	2.3
L130	HD11	2.6
L130	HD22	2.3
L130	HD21	2.8
L130	HB1	3.1
L130	CD1	3.3
L130	HB1	2.8
L130	HD13	2.4
L130	HD22	2.8
E131	O	3.5
E131	O	2.9
C133	O	1.8
C133	O	3.4
C133	H	3.5
C133	O	2.8
C133	O	3.4
C133	H	3.5
C133	C	3.0

C133	O	1.8
C133	O	2.6
R134	HA	3.2
R134	CA	3.3
R134	HA	2.3
R135	HH22	2.0
R135	H	3.2
R135	HB1	3.4
R135	CZ	3.5
R135	NH1	3.4
R135	NH2	2.9
R135	HH11	2.8
R135	HH22	2.0
R135	H	3.5
R135	NH2	3.4
R135	HH11	3.1
R135	HH22	2.8
R135	NH1	3.3
R135	HH11	2.9
R135	H	2.9
R135	H	3.5
R135	HH11	3.3
R135	HH22	2.8
R135	NH1	2.9
R135	HH12	3.2
R135	HH11	2.4
F183	HZ	3.5
F183	HZ	3.3
F183	HE1	3.2
F183	HZ	3.4
F183	CE1	3.3
F183	HE1	3.0
F183	CE1	3.4
F183	HE1	2.8
F183	HE1	2.9
F183	HE1	3.3
F183	HE2	3.1
F183	HD1	3.3
F183	HE1	3.2
F183	HE1	3.4
G193	HA2	3.3
D194	OD2	3.5
D194	OD1	3.1
D194	OD2	3.4
D194	H	3.2
D194	CG	2.9

D194	OD1	2.5
D194	OD2	2.6
D194	N	3.0
D194	H	2.7
D194	H	3.4
D194	N	3.1
D194	CA	3.3
D194	CG	3.0
D194	OD1	2.6
D194	H	2.7
D194	HA	2.7

Table 12. In vitro activity of flavonoid compounds

No	Inhibitor	Plk1 IC_{50} (μM)	PI3K IC50 (μM)	CDK2 IC50 (μM)
1	Wortmannin	0.18±0.1	0.0042	>10
2	Staurosporine	0.8±0.2	9	0.004
3	Purvalanol A	5	ND	0.0009±0.002
4	LY2940002	9.33±3.7	1.4	ND
5	Quercetin	64.25±24	3.8	ND

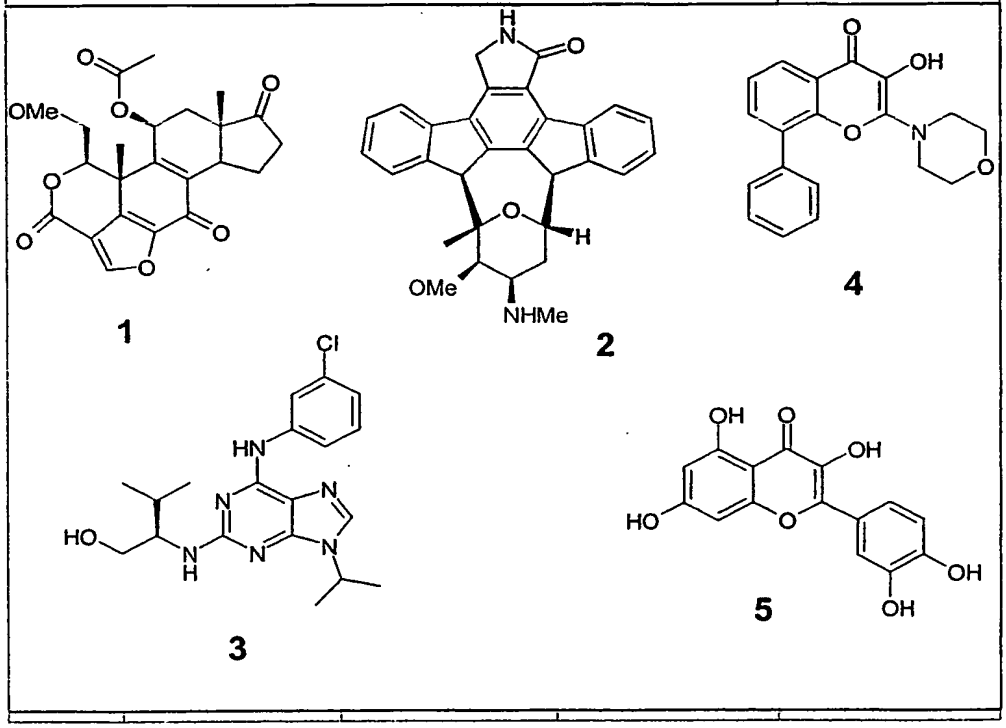


Table 13. In vitro potencies for flavonoid compounds.

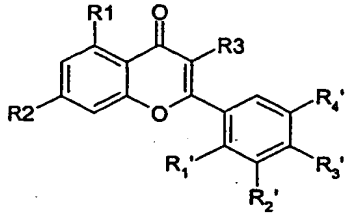
	Structure							Kinase inhibition (μM)
								
	R^1	R^2	R^3	R1'	R2'	R3'	R4'	Plk1 IC_{50} (μM)
Morin Hydrate	OH	OH	OH	OH	H	OH	H	12.6±1.4
Datescetin	OH	OH	OH	OH	H	H	H	>100
Quercetin	OH	OH	OH	H	OH	OH	H	64.25±24
Myricetin	OH	OH	OH	H	OH	OH	OH	>100
Kaempferol	OH	OH	OH	H	H	OH	H	>100
Luteolin	OH	OH	H	H	OH	OH	H	>100
Galangin	OH	OH	OH	H	H	H	H	>100
Robinetin	H	OH	OH	H	OH	OH	OH	60
Daidzein	H	OH	H	H	H	OH	H	>100
Fisetin	H	OH	OH	H	OH	OH	H	>100
Kaempferide	OH	OH	OH	H	H	Ome	H	>100

Table 14. In vitro testing of PKA inhibitors

Compound	PKA (IC50, μM)	Plk1 (IC50, μM)
Balanol	0.003, 0.004*	>200
H89	0.048**	>500
A3	11**	>500
puravalanol A	>100	10
4-Cyano-3-methylisoquinoline	0.030**	>500
KT5720	0.056**	>500